

Sample name: **M09_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03001**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 12:18:26 AM**
 Analyst: **Pion**
 Instrument ID: **T312060**

pH-metric Result

logP (XH +) 1.05 ±0.04 (n=50)
 logP (neutral X) 3.14 ±0.01 (n=50)

18C-03001 Points 1 to 25

M09_octanol concentration factor 1.208
 Carbonate 0.0513 mM
 Acidity error -0.65776 mM

18C-03001 Points 26 to 53

M09_octanol concentration factor 1.218
 Carbonate 0.1056 mM
 Acidity error -0.76829 mM

18C-03001 Points 54 to 80

M09_octanol concentration factor 1.072
 Carbonate 0.0742 mM
 Acidity error -0.32205 mM

Warnings and errors

Errors None
 Warnings None

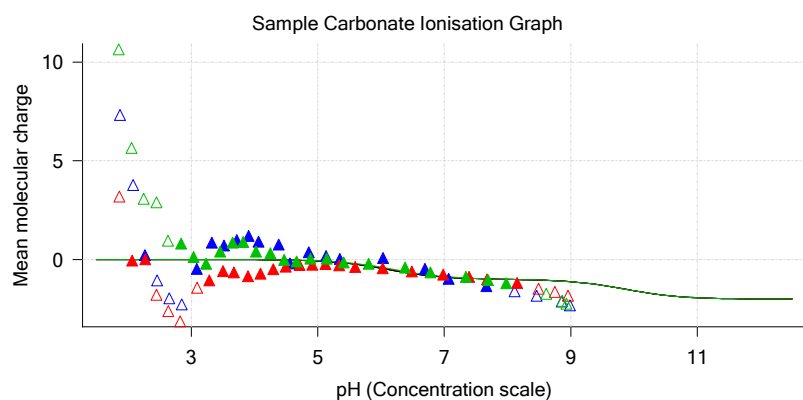
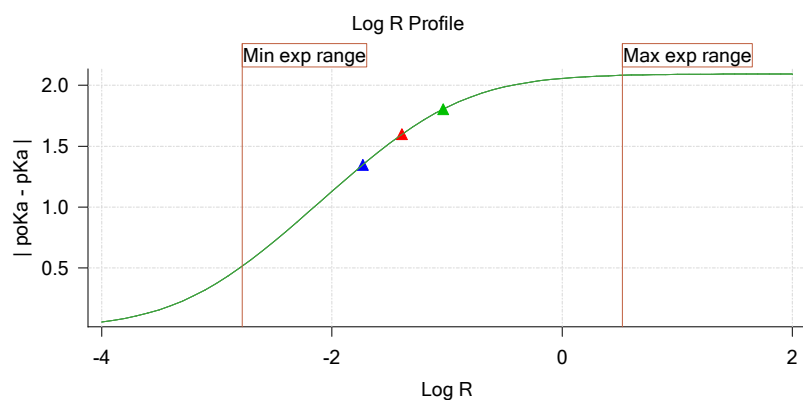
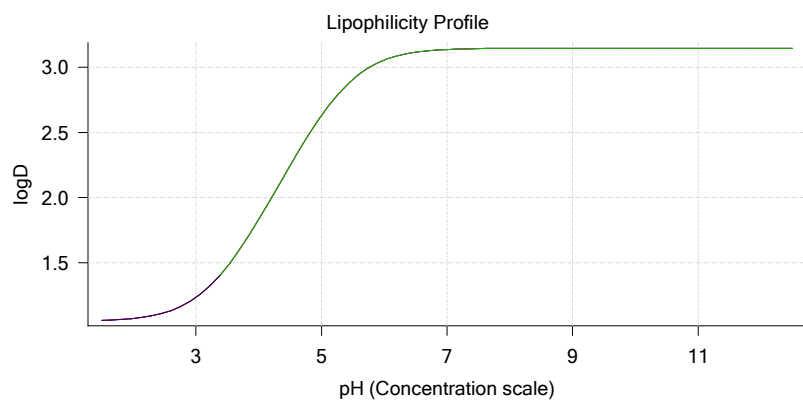
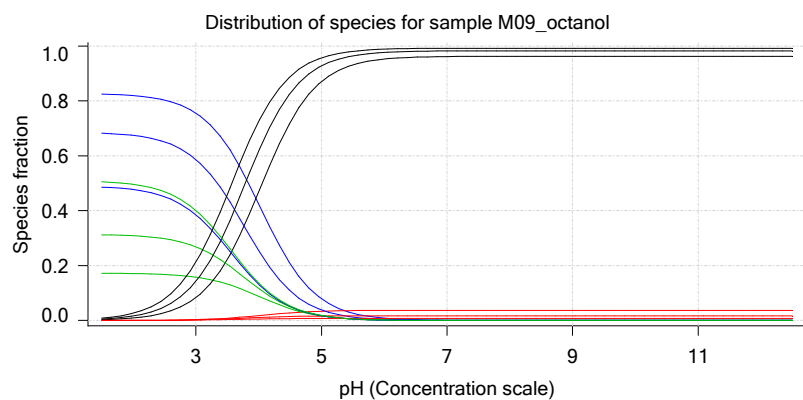
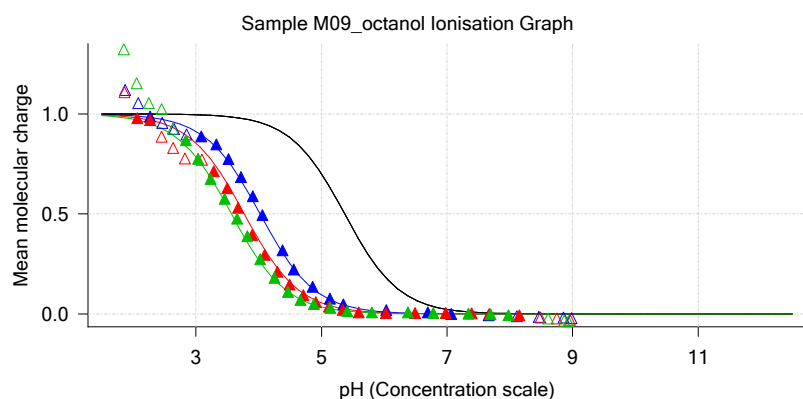
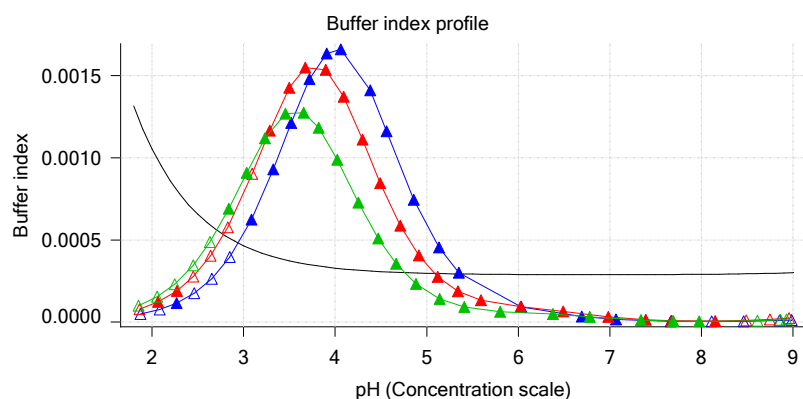
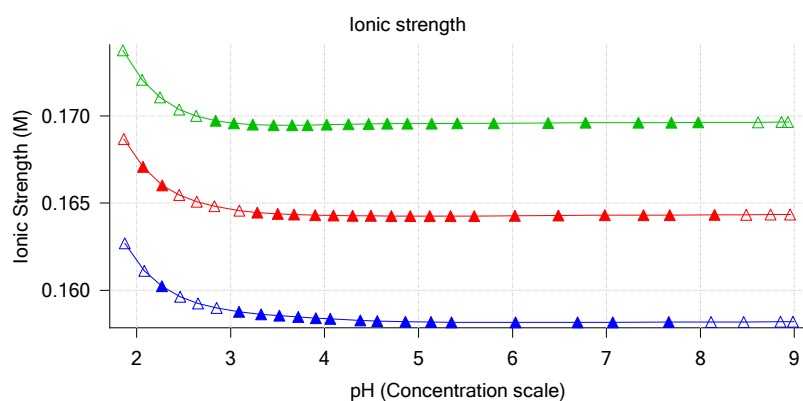
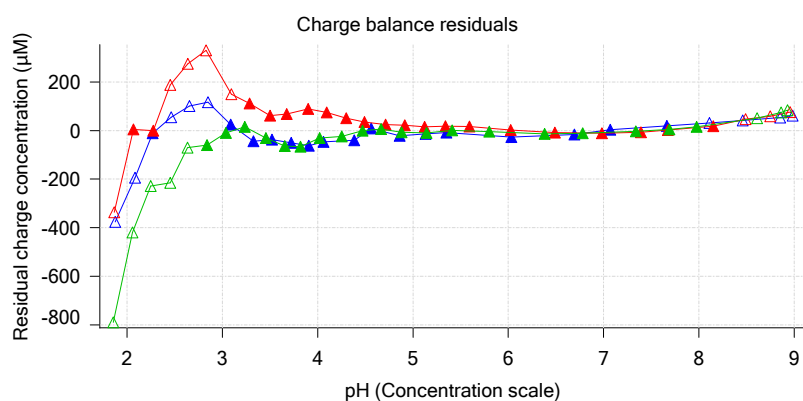
Sample logD and percent species

pH	M09_octanol logD	M09_octanol M09_octanolH	M09_octanol M09_octanol	M09_octanol M09_octanolH*	M09_octanol M09_octanol*	Comment
1.000	1.05	8.12 %	0.00 %	91.40 %	0.48 %	Stomach pH
1.200	1.05	8.10 %	0.00 %	91.14 %	0.76 %	
2.000	1.07	7.78 %	0.00 %	87.58 %	4.63 %	
3.000	1.23	5.49 %	0.02 %	61.80 %	32.69 %	
4.000	1.83	1.39 %	0.06 %	15.67 %	82.88 %	
5.000	2.63	0.16 %	0.07 %	1.85 %	97.91 %	Blood pH
6.000	3.05	0.02 %	0.07 %	0.19 %	99.72 %	
6.500	3.11	0.01 %	0.07 %	0.06 %	99.86 %	
7.000	3.13	0.00 %	0.07 %	0.02 %	99.91 %	
7.400	3.14	0.00 %	0.07 %	0.01 %	99.92 %	
8.000	3.14	0.00 %	0.07 %	0.00 %	99.93 %	
9.000	3.14	0.00 %	0.07 %	0.00 %	99.93 %	
10.000	3.14	0.00 %	0.07 %	0.00 %	99.93 %	
11.000	3.14	0.00 %	0.07 %	0.00 %	99.93 %	
12.000	3.14	0.00 %	0.07 %	0.00 %	99.93 %	

Sample name: **M09_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03001**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 12:18:26 AM**
 Analyst: **Pion**
 Instrument ID: **T312060**

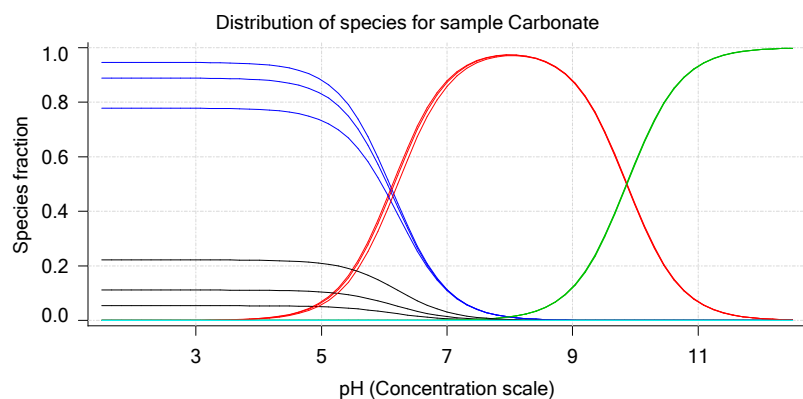
Graphs



Sample name: **M09_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03001**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 12:18:26 AM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Graphs (continued)



Sample name: **M09_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03001**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 12:18:26 AM**
 Analyst: **Pion**
 Instrument ID: **T312060**

pH-metric high logP Titration 1 of 3 18C-03001 Points 1 to 25

Overall results

RMSD 0.656
 Average ionic strength 0.158 M
 Average temperature 25.0°C
 Partition ratio 0.0185 : 1
 Analyte concentration range 2340.8 µM to 2417.9 µM
 Total points considered 16 of 25

Warnings and errors

Errors None
 Warnings None

Four-Plus parameters

Alpha 0.111 3/3/2018 12:18:25 AM C:\Sirius_T3\HCl18C02.t3r
 S 0.9988 3/3/2018 12:18:25 AM C:\Sirius_T3\HCl18C02.t3r
 jH 1.0 3/3/2018 12:18:25 AM C:\Sirius_T3\HCl18C02.t3r
 jOH -0.8 3/3/2018 12:18:25 AM C:\Sirius_T3\HCl18C02.t3r

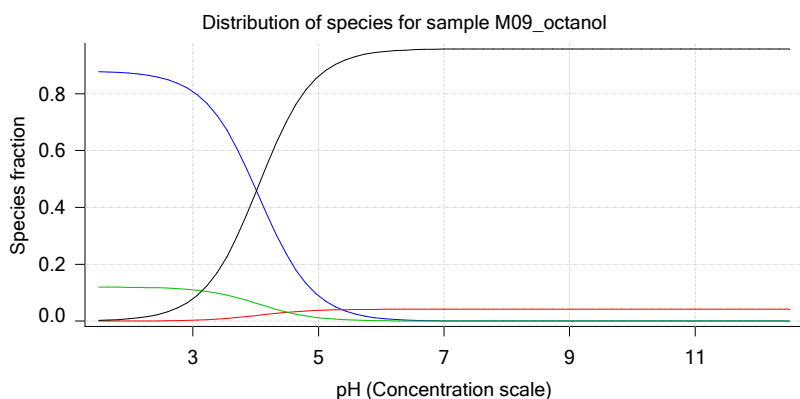
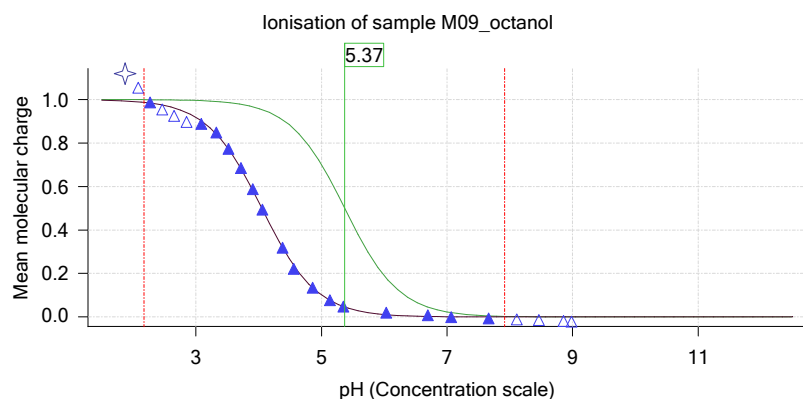
Titrants

0.50 M HCl 0.999058 3/3/2018 12:18:25 AM C:\Sirius_T3\HCl18C02.t3r
 0.50 M KOH 0.999845 3/3/2018 12:18:26 AM C:\Sirius_T3\KOH18B27.t3r

Sample

M09_octanol concentration factor 1.208
 M09_octanol stoichiometry 1.000
 Chloride stoichiometry 1.000
 Base pKa 1 5.37
 logP (XH +) 0.87
 logP (neutral X) 3.09

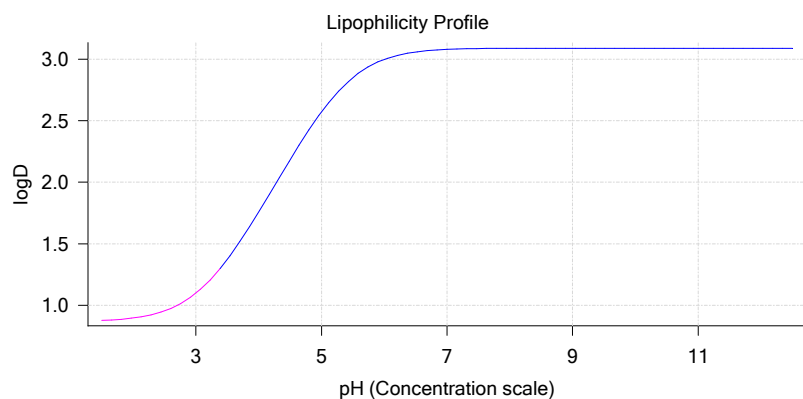
Sample graphs



Sample name: **M09_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03001**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 12:18:26 AM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Sample graphs (continued)



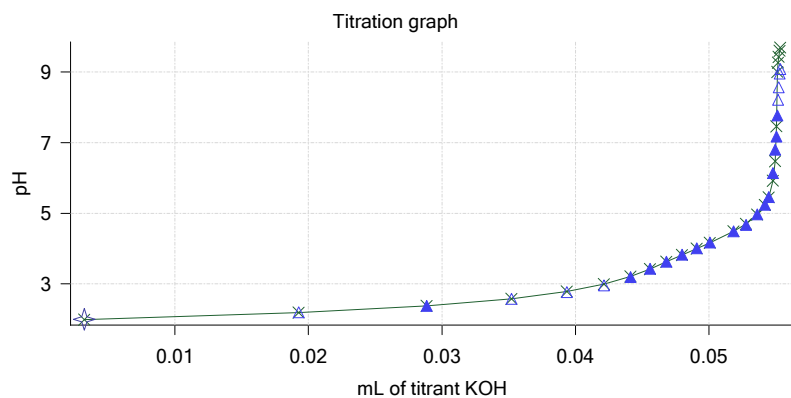
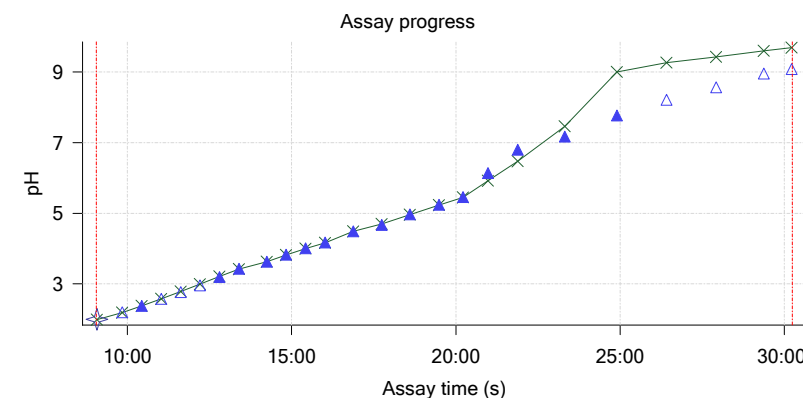
Sample logD and percent species

pH	M09_octanol logD	M09_octanol M09_octanolH	M09_octanol M09_octanolH	M09_octanol M09_octanolH*	M09_octanol M09_octanol*	Comment
1.000	0.87	87.91 %	0.00 %	12.00 %	0.09 %	
1.200	0.87	87.86 %	0.01 %	12.00 %	0.13 %	
2.000	0.90	87.21 %	0.04 %	11.91 %	0.84 %	
3.000	1.10	80.80 %	0.34 %	11.03 %	7.83 %	
4.000	1.76	46.56 %	1.99 %	6.36 %	45.10 %	
5.000	2.57	8.89 %	3.79 %	1.21 %	86.10 %	
6.000	3.00	0.98 %	4.17 %	0.13 %	94.72 %	
6.500	3.06	0.31 %	4.20 %	0.04 %	95.44 %	
7.000	3.08	0.10 %	4.21 %	0.01 %	95.67 %	
7.400	3.08	0.04 %	4.22 %	0.01 %	95.74 %	
8.000	3.09	0.01 %	4.22 %	0.00 %	95.77 %	
9.000	3.09	0.00 %	4.22 %	0.00 %	95.78 %	
10.000	3.09	0.00 %	4.22 %	0.00 %	95.78 %	
11.000	3.09	0.00 %	4.22 %	0.00 %	95.78 %	
12.000	3.09	0.00 %	4.22 %	0.00 %	95.78 %	

Carbonate and acidity

Carbonate 0.051 mM
 Acidity error -0.658 mM

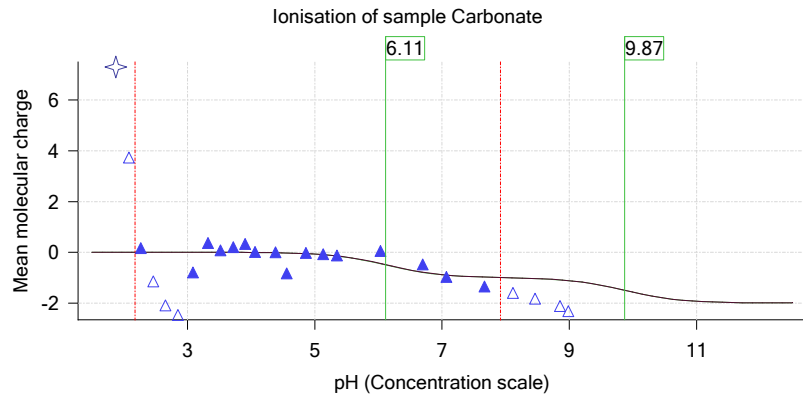
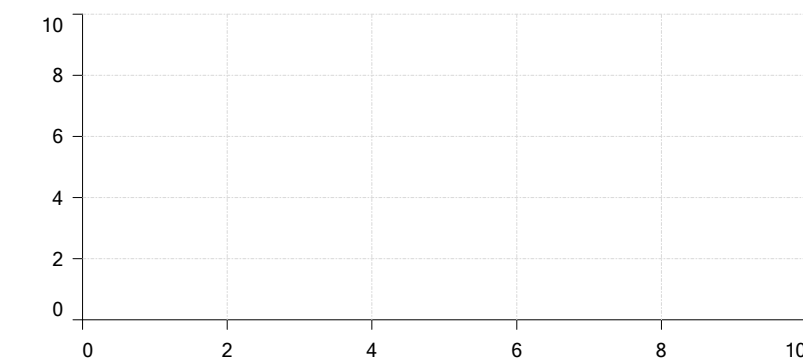
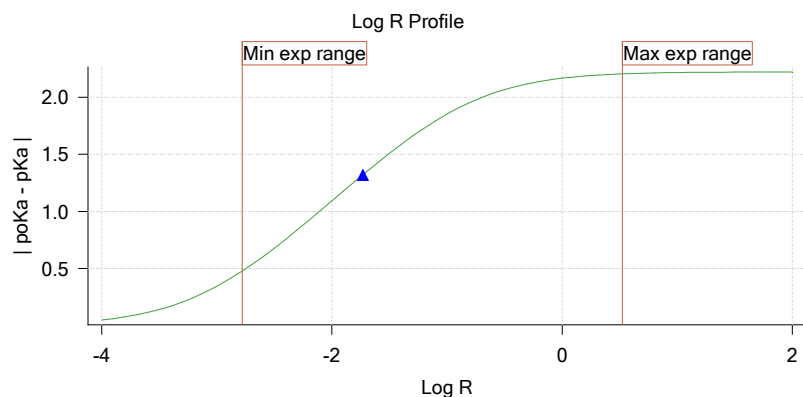
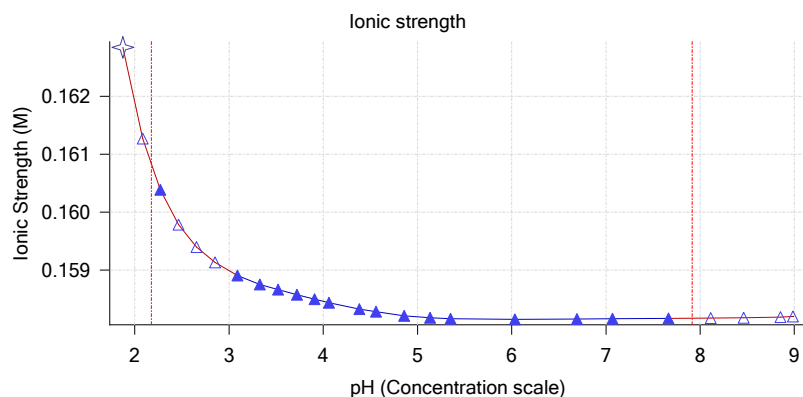
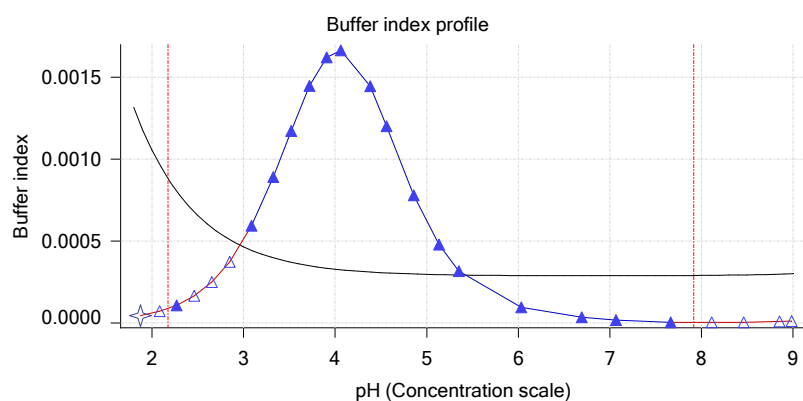
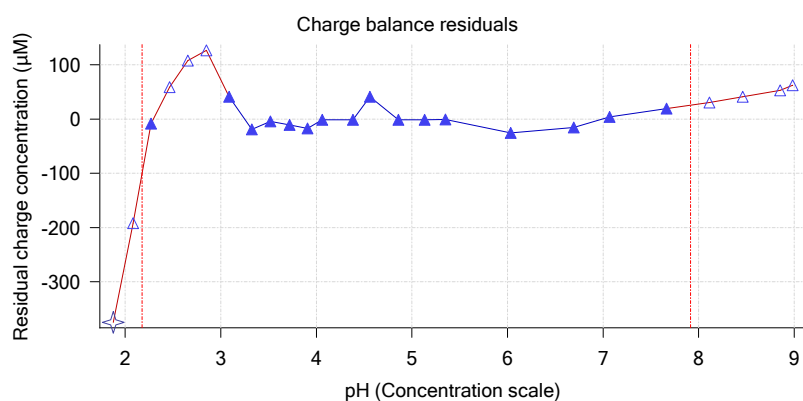
Other graphs



Sample name: **M09_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03001**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 12:18:26 AM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Other graphs (continued)



Sample name: **M09_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03001**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 12:18:26 AM**
 Analyst: **Pion**
 Instrument ID: **T312060**

pH-metric high logP Titration 2 of 3 18C-03001 Points 26 to 53

Overall results

RMSD 0.344
 Average ionic strength 0.165 M
 Average temperature 25.0°C
 Partition ratio 0.0407 : 1
 Analyte concentration range 2140.2 µM to 2210.0 µM
 Total points considered 20 of 28

Warnings and errors

Errors None
 Warnings None

Four-Plus parameters

Alpha 0.111 3/3/2018 12:18:25 AM C:\Sirius_T3\HCl18C02.t3r
 S 0.9988 3/3/2018 12:18:25 AM C:\Sirius_T3\HCl18C02.t3r
 jH 1.0 3/3/2018 12:18:25 AM C:\Sirius_T3\HCl18C02.t3r
 jOH -0.8 3/3/2018 12:18:25 AM C:\Sirius_T3\HCl18C02.t3r

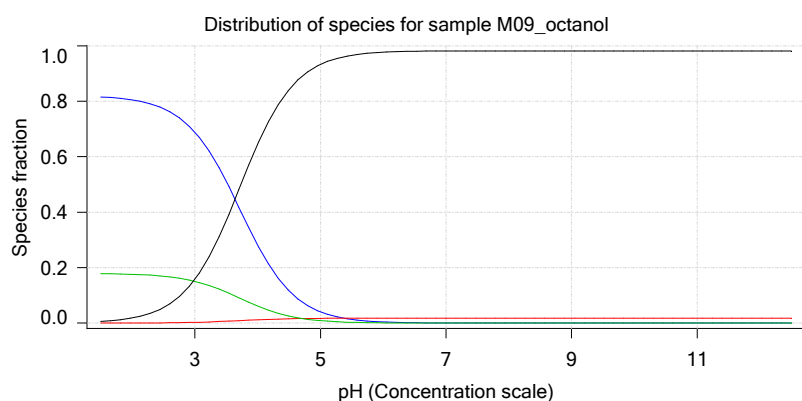
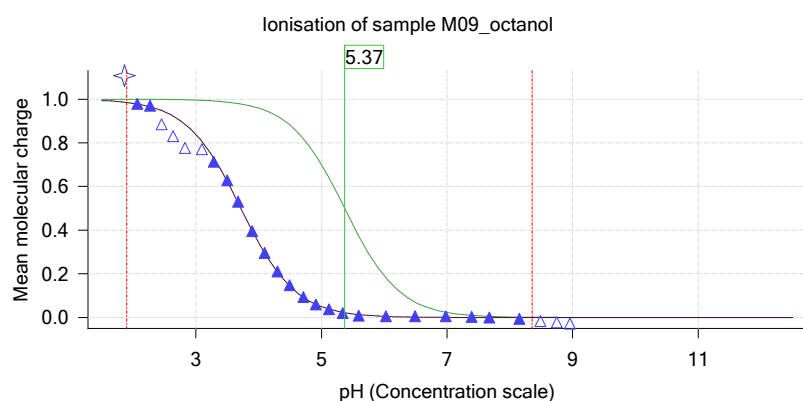
Titrants

0.50 M HCl 0.999058 3/3/2018 12:18:25 AM C:\Sirius_T3\HCl18C02.t3r
 0.50 M KOH 0.999845 3/3/2018 12:18:26 AM C:\Sirius_T3\KOH18B27.t3r

Sample

M09_octanol concentration factor 1.218
 M09_octanol stoichiometry 1.000
 Chloride stoichiometry 1.000
 Base pKa 1 5.37
 logP (XH +) 0.73
 logP (neutral X) 3.12

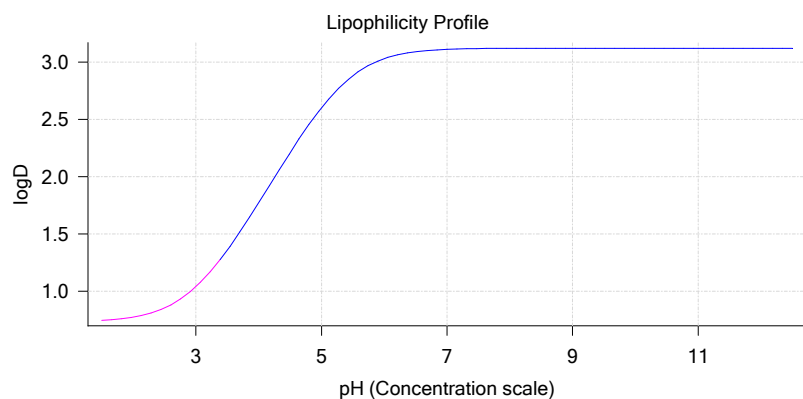
Sample graphs



Sample name: **M09_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03001**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 12:18:26 AM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Sample graphs (continued)



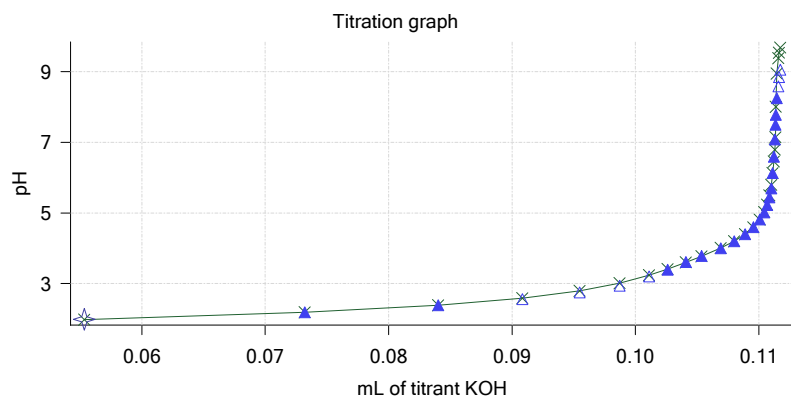
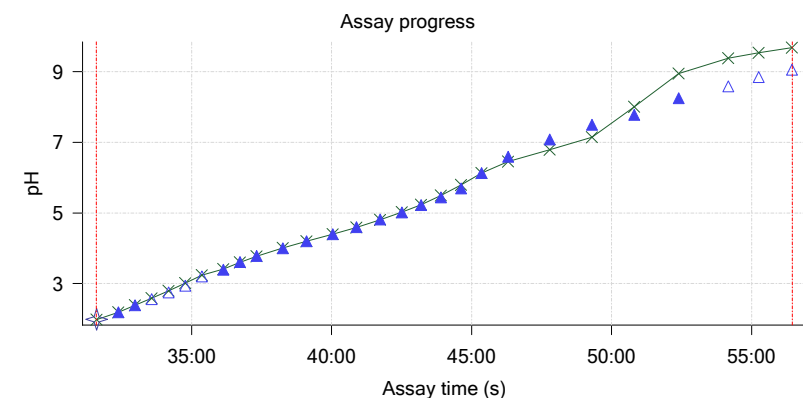
Sample logD and percent species

pH	M09_octanol logD	M09_octanol M09_octanolH	M09_octanol M09_octanolH	M09_octanol M09_octanolH*	M09_octanol M09_octanol*	Comment
1.000	0.74	81.90 %	0.00 %	17.91 %	0.19 %	
1.200	0.74	81.80 %	0.01 %	17.89 %	0.30 %	
2.000	0.77	80.51 %	0.03 %	17.61 %	1.85 %	
3.000	1.04	68.86 %	0.29 %	15.06 %	15.78 %	
4.000	1.77	28.14 %	1.20 %	6.16 %	64.50 %	
5.000	2.60	4.07 %	1.74 %	0.89 %	93.30 %	
6.000	3.03	0.43 %	1.82 %	0.09 %	97.66 %	
6.500	3.09	0.14 %	1.82 %	0.03 %	98.01 %	
7.000	3.11	0.04 %	1.83 %	0.01 %	98.12 %	
7.400	3.12	0.02 %	1.83 %	0.00 %	98.15 %	
8.000	3.12	0.00 %	1.83 %	0.00 %	98.17 %	
9.000	3.12	0.00 %	1.83 %	0.00 %	98.17 %	
10.000	3.12	0.00 %	1.83 %	0.00 %	98.17 %	
11.000	3.12	0.00 %	1.83 %	0.00 %	98.17 %	
12.000	3.12	0.00 %	1.83 %	0.00 %	98.17 %	

Carbonate and acidity

Carbonate 0.106 mM
 Acidity error -0.768 mM

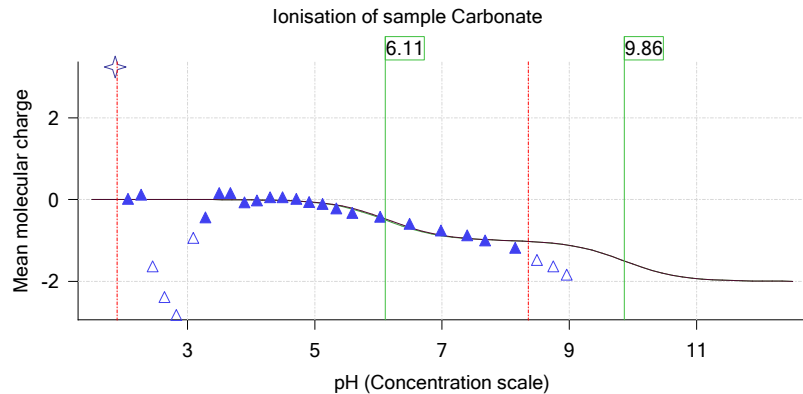
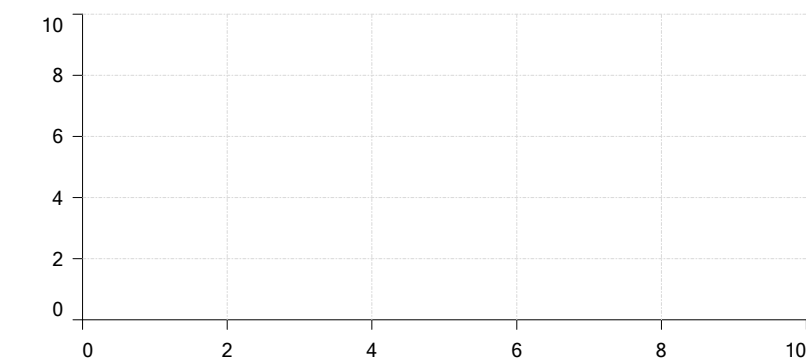
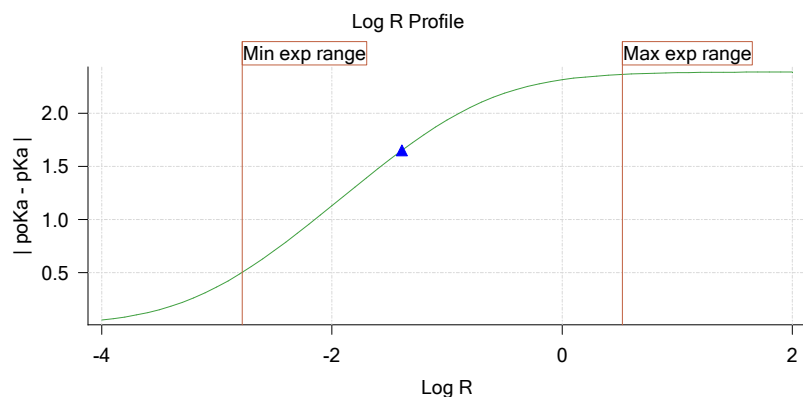
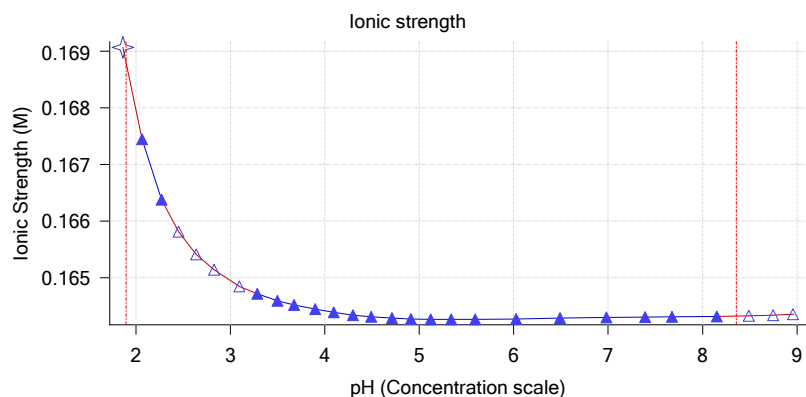
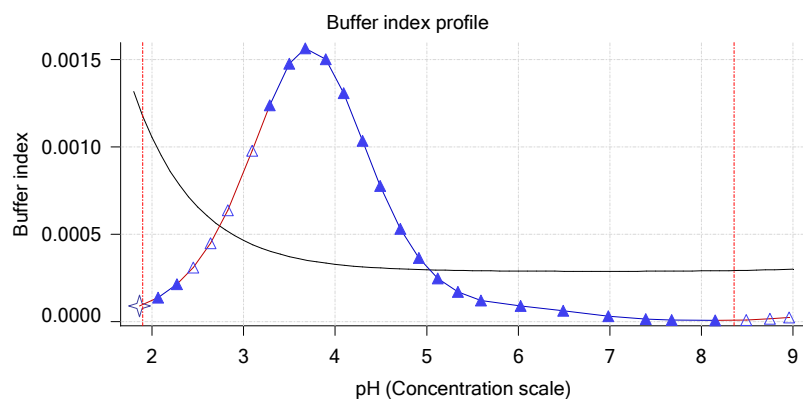
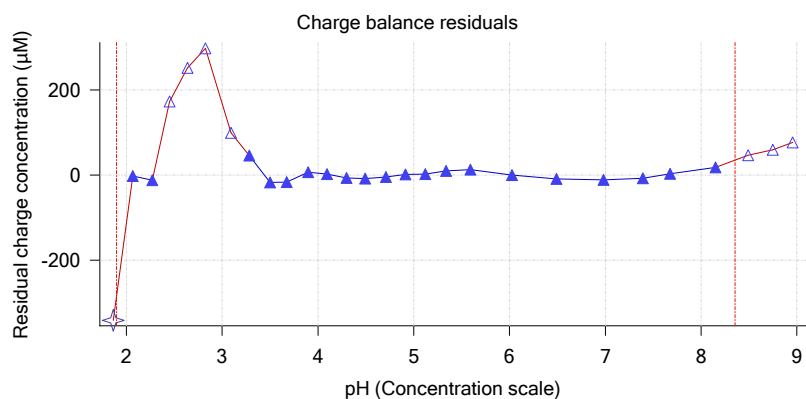
Other graphs



Sample name: **M09_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03001**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 12:18:26 AM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Other graphs (continued)



Sample name: **M09_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03001**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 12:18:26 AM**
 Analyst: **Pion**
 Instrument ID: **T312060**

pH-metric high logP Titration 3 of 3 18C-03001 Points 54 to 80

Overall results

RMSD 0.436
 Average ionic strength 0.170 M
 Average temperature 25.0°C
 Partition ratio 0.0924 : 1
 Analyte concentration range 1903.5 µM to 1963.3 µM
 Total points considered 19 of 27

Warnings and errors

Errors None
 Warnings None

Four-Plus parameters

Alpha 0.111 3/3/2018 12:18:25 AM C:\Sirius_T3\HCl18C02.t3r
 S 0.9988 3/3/2018 12:18:25 AM C:\Sirius_T3\HCl18C02.t3r
 jH 1.0 3/3/2018 12:18:25 AM C:\Sirius_T3\HCl18C02.t3r
 jOH -0.8 3/3/2018 12:18:25 AM C:\Sirius_T3\HCl18C02.t3r

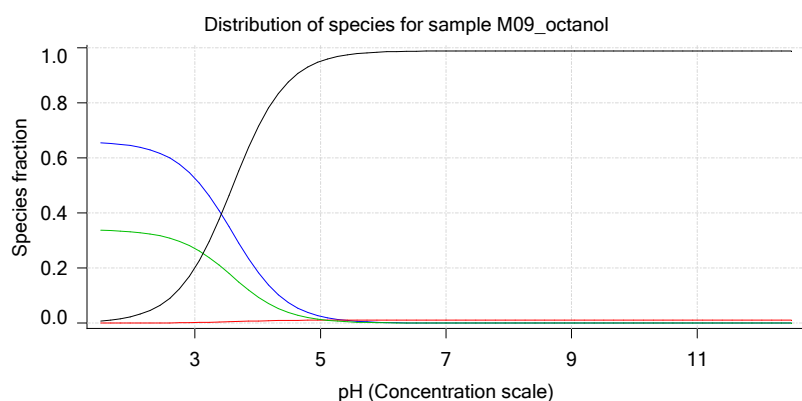
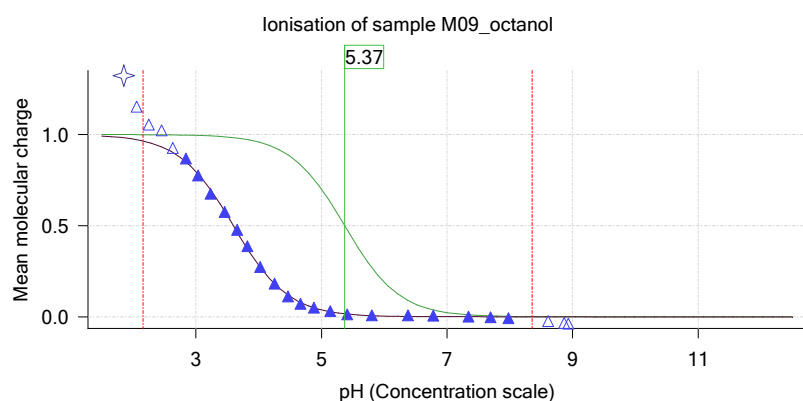
Titrants

0.50 M HCl 0.999058 3/3/2018 12:18:25 AM C:\Sirius_T3\HCl18C02.t3r
 0.50 M KOH 0.999845 3/3/2018 12:18:26 AM C:\Sirius_T3\KOH18B27.t3r

Sample

M09_octanol concentration factor 1.072
 M09_octanol stoichiometry 1.000
 Chloride stoichiometry 1.000
 Base pKa 1 5.37
 logP (XH +) 0.75
 logP (neutral X) 2.98

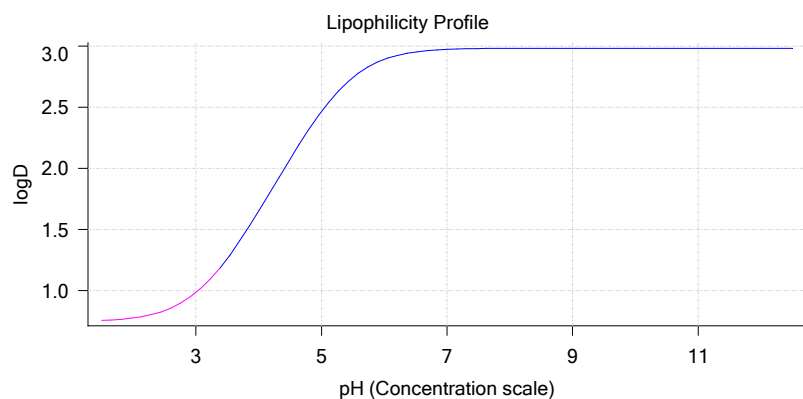
Sample graphs



Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03001**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 12:18:26 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)



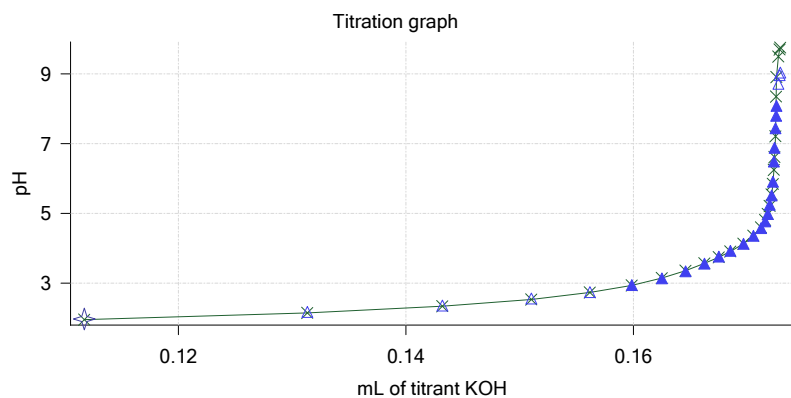
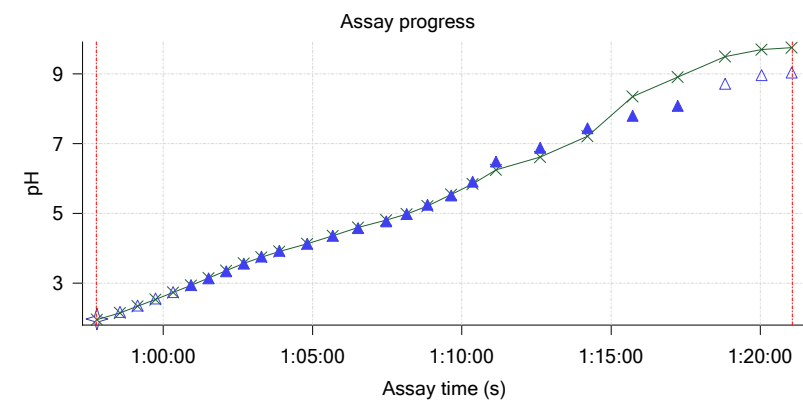
Sample logD and percent species

pH	M09_octanol logD	M09_octanol M09_octanolH	M09_octanol M09_octanolH	M09_octanol M09_octanolH*	M09_octanol M09_octanol*	Comment
1.000	0.75	65.86 %	0.00 %	33.89 %	0.25 %	Stomach pH
1.200	0.75	65.76 %	0.00 %	33.84 %	0.40 %	
2.000	0.78	64.40 %	0.03 %	33.13 %	2.44 %	
3.000	0.98	52.69 %	0.22 %	27.11 %	19.97 %	
4.000	1.65	18.70 %	0.80 %	9.62 %	70.88 %	
5.000	2.46	2.51 %	1.07 %	1.29 %	95.13 %	Blood pH
6.000	2.89	0.26 %	1.11 %	0.13 %	98.50 %	
6.500	2.95	0.08 %	1.11 %	0.04 %	98.76 %	
7.000	2.97	0.03 %	1.11 %	0.01 %	98.85 %	
7.400	2.98	0.01 %	1.11 %	0.01 %	98.87 %	
8.000	2.98	0.00 %	1.11 %	0.00 %	98.88 %	
9.000	2.98	0.00 %	1.11 %	0.00 %	98.89 %	
10.000	2.98	0.00 %	1.11 %	0.00 %	98.89 %	
11.000	2.98	0.00 %	1.11 %	0.00 %	98.89 %	
12.000	2.98	0.00 %	1.11 %	0.00 %	98.89 %	

Carbonate and acidity

Carbonate 0.074 mM
Acidity error -0.322 mM

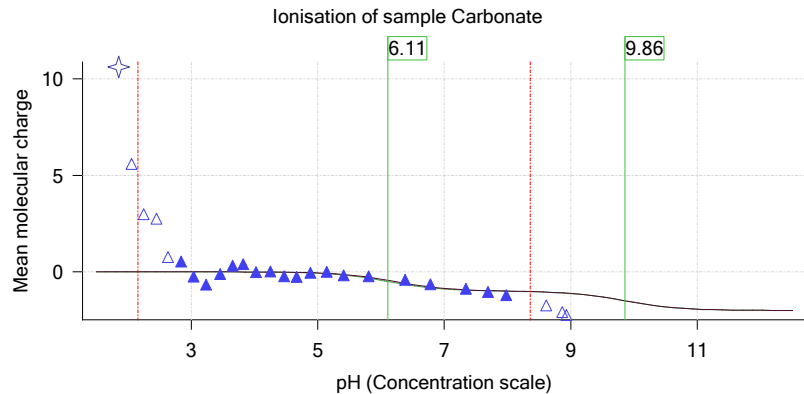
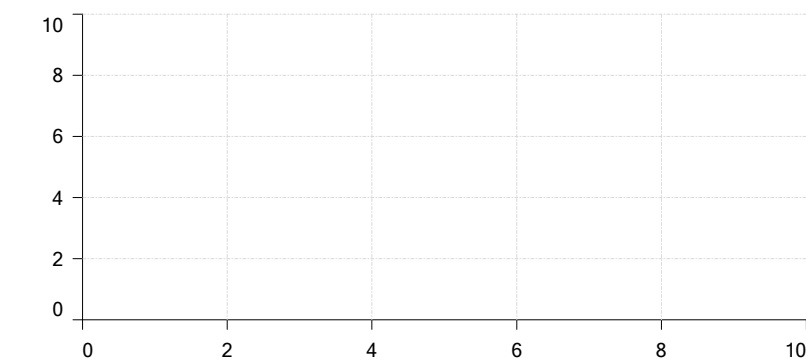
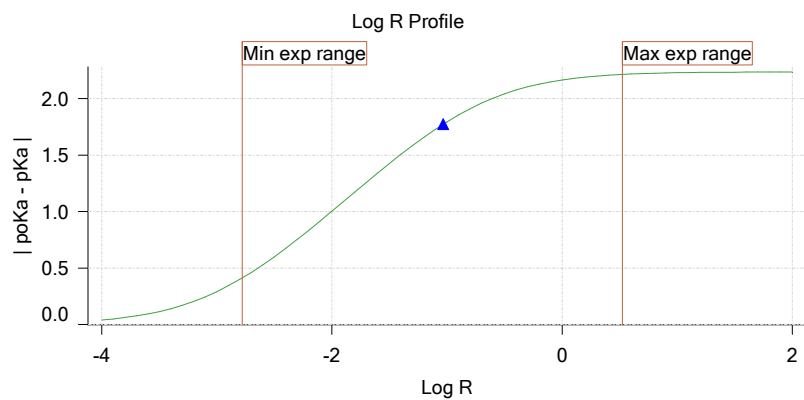
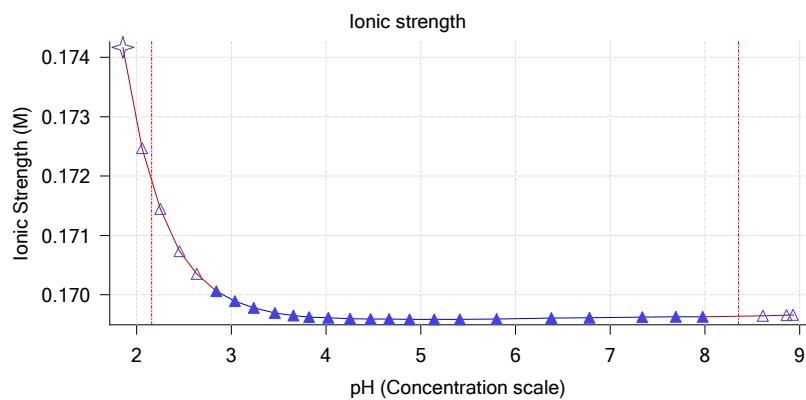
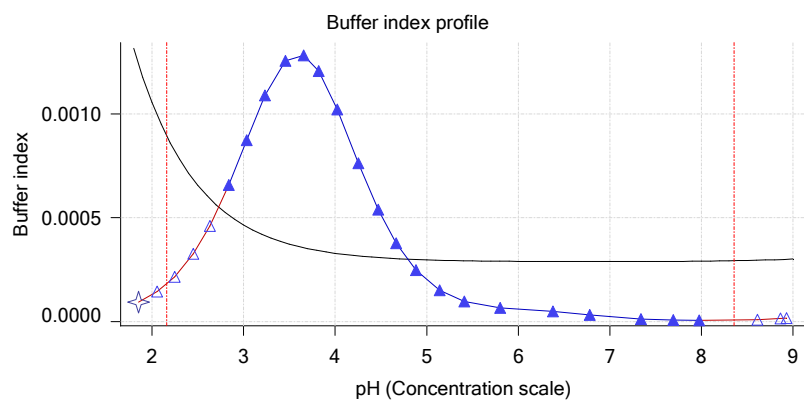
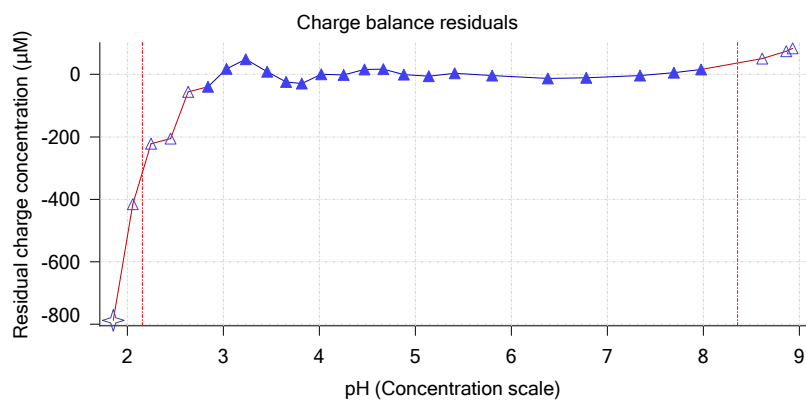
Other graphs



Sample name: **M09_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03001**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 12:18:26 AM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Other graphs (continued)



Sample name: **M09_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03001**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 12:18:26 AM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M09_octanol	2/27/2018 4:56:17 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.001100 g	3/2/2018 5:08:41 PM	User entered value
Formula weight	287.74 g/mol	2/27/2018 4:45:45 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	251.28	2/27/2018 4:45:45 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	2/27/2018 4:45:45 PM	User entered value
Sample is a	Base	2/27/2018 4:45:45 PM	User entered value
pKa 1	5.37	2/27/2018 4:45:45 PM	User entered value
logp (XH +)	0.76	3/2/2018 3:27:23 PM	User entered value
logP (neutral X)	3.27	3/2/2018 3:27:17 PM	User entered value
Stoichiometry	1.00000		Default value
Aprotic counterion name	Chloride		From standards.xml file
Stoichiometry	1.00		From standards.xml file
Charge per counterion	-1		From standards.xml file

Events

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
5:59.7	Initial pH = 4.70									
9:04.4	Data point 1	1.50000 mL	0.04781 mL	0.00322 mL	0.03001 mL	1.997	0.00021	0.00128	0.00028	10.0 s
9:50.6	Data point 2	1.50000 mL	0.04781 mL	0.01929 mL	0.03001 mL	2.199	-0.00807	0.15986	0.00100	10.0 s
10:26.3	Data point 3	1.50000 mL	0.04781 mL	0.02886 mL	0.03001 mL	2.383	-0.00750	0.76284	0.00042	10.0 s
11:01.9	Data point 4	1.50000 mL	0.04781 mL	0.03521 mL	0.03001 mL	2.574	-0.00115	0.21590	0.00012	10.0 s
11:37.4	Data point 5	1.50000 mL	0.04781 mL	0.03935 mL	0.03001 mL	2.764	-0.00311	0.44869	0.00023	10.0 s
12:12.9	Data point 6	1.50000 mL	0.04781 mL	0.04214 mL	0.03001 mL	2.959	0.00347	0.05811	0.00071	10.0 s
12:48.4	Data point 7	1.50000 mL	0.04781 mL	0.04412 mL	0.03001 mL	3.196	-0.00193	0.10328	0.00030	10.0 s
13:23.8	Data point 8	1.50000 mL	0.04781 mL	0.04558 mL	0.03001 mL	3.433	-0.00576	0.33769	0.00049	10.0 s
14:14.7	Data point 9	1.50000 mL	0.04781 mL	0.04680 mL	0.03001 mL	3.626	0.00424	0.07343	0.00077	10.0 s
14:50.2	Data point 10	1.50000 mL	0.04781 mL	0.04798 mL	0.03001 mL	3.827	-0.00743	0.22433	0.00078	10.0 s
15:25.6	Data point 11	1.50000 mL	0.04781 mL	0.04908 mL	0.03001 mL	4.012	-0.00611	0.18146	0.00071	10.0 s
16:01.0	Data point 12	1.50000 mL	0.04781 mL	0.05007 mL	0.03001 mL	4.168	0.00689	0.18082	0.00080	10.5 s
16:52.5	Data point 13	1.50000 mL	0.04781 mL	0.05183 mL	0.03001 mL	4.487	0.00440	0.05974	0.00089	11.0 s
17:44.4	Data point 14	1.50000 mL	0.04781 mL	0.05278 mL	0.03001 mL	4.667	-0.01155	0.70656	0.00068	11.0 s
18:36.3	Data point 15	1.50000 mL	0.04781 mL	0.05362 mL	0.03001 mL	4.964	-0.01372	0.57218	0.00090	12.0 s
19:29.2	Data point 16	1.50000 mL	0.04781 mL	0.05419 mL	0.03001 mL	5.238	-0.01399	0.63621	0.00087	13.5 s
20:13.3	Data point 17	1.50000 mL	0.04781 mL	0.05447 mL	0.03001 mL	5.454	-0.01800	0.81818	0.00098	14.5 s
20:58.4	Data point 18	1.50000 mL	0.04781 mL	0.05480 mL	0.03001 mL	6.136	-0.01947	0.94607	0.00099	24.0 s
21:53.1	Data point 19	1.50000 mL	0.04781 mL	0.05496 mL	0.03001 mL	6.796	-0.01955	0.98614	0.00097	55.0 s
23:18.9	Data point 20	1.50000 mL	0.04781 mL	0.05506 mL	0.03001 mL	7.170	-0.02220	0.96314	0.00112	Timed out at 59.5 s
24:54.4	Data point 21	1.50000 mL	0.04781 mL	0.05513 mL	0.03001 mL	7.765	-0.05086	0.98182	0.00253	Timed out at 59.5 s
26:24.9	Data point 22	1.50000 mL	0.04781 mL	0.05517 mL	0.03001 mL	8.213	-0.03736	0.98947	0.00186	Timed out at 59.5 s
27:55.4	Data point 23	1.50000 mL	0.04781 mL	0.05522 mL	0.03001 mL	8.561	-0.01843	0.94257	0.00094	51.0 s
29:22.2	Data point 24	1.50000 mL	0.04781 mL	0.05529 mL	0.03001 mL	8.953	-0.01480	0.58788	0.00095	20.5 s
30:13.4	Data point 25	1.50000 mL	0.04781 mL	0.05534 mL	0.03001 mL	9.083	-0.01975	0.98237	0.00098	24.0 s
31:36.5	Data point 26	1.50000 mL	0.10442 mL	0.05534 mL	0.07001 mL	1.986	-0.00842	0.45051	0.00062	10.0 s
32:22.8	Data point 27	1.50000 mL	0.10442 mL	0.07321 mL	0.07001 mL	2.184	0.00425	0.08074	0.00074	10.0 s
32:58.4	Data point 28	1.50000 mL	0.10442 mL	0.08401 mL	0.07001 mL	2.386	-0.00574	0.55446	0.00038	10.5 s
33:34.5	Data point 29	1.50000 mL	0.10442 mL	0.09083 mL	0.07001 mL	2.563	-0.00261	0.29606	0.00024	10.5 s
34:10.6	Data point 30	1.50000 mL	0.10442 mL	0.09548 mL	0.07001 mL	2.748	-0.00851	0.22823	0.00088	10.0 s
34:46.1	Data point 31	1.50000 mL	0.10442 mL	0.09873 mL	0.07001 mL	2.936	-0.00490	0.63259	0.00030	10.0 s
35:21.6	Data point 32	1.50000 mL	0.10442 mL	0.10111 mL	0.07001 mL	3.202	0.00315	0.37649	0.00025	10.5 s
36:07.9	Data point 33	1.50000 mL	0.10442 mL	0.10261 mL	0.07001 mL	3.392	-0.00411	0.37428	0.00033	10.0 s

Sample name: **M09_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03001**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 12:18:26 AM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
36:43.4	Data point 34	1.50000 mL	0.10442 mL	0.10409 mL	0.07001 mL	3.607	-0.00351	0.55022	0.00023	10.0 s
37:18.9	Data point 35	1.50000 mL	0.10442 mL	0.10536 mL	0.07001 mL	3.781	-0.00697	0.45953	0.00051	10.0 s
38:15.1	Data point 36	1.50000 mL	0.10442 mL	0.10691 mL	0.07001 mL	4.005	0.00441	0.11123	0.00065	10.5 s
39:06.5	Data point 37	1.50000 mL	0.10442 mL	0.10800 mL	0.07001 mL	4.199	-0.00237	0.07863	0.00042	10.0 s
40:02.4	Data point 38	1.50000 mL	0.10442 mL	0.10889 mL	0.07001 mL	4.404	-0.00334	0.17918	0.00039	10.0 s
40:53.4	Data point 39	1.50000 mL	0.10442 mL	0.10955 mL	0.07001 mL	4.598	-0.01051	0.50833	0.00073	10.0 s
41:44.3	Data point 40	1.50000 mL	0.10442 mL	0.11009 mL	0.07001 mL	4.816	-0.00546	0.23998	0.00055	10.5 s
42:30.4	Data point 41	1.50000 mL	0.10442 mL	0.11044 mL	0.07001 mL	5.018	-0.00850	0.19854	0.00094	11.0 s
43:12.0	Data point 42	1.50000 mL	0.10442 mL	0.11068 mL	0.07001 mL	5.225	-0.01559	0.61445	0.00098	11.5 s
43:54.1	Data point 43	1.50000 mL	0.10442 mL	0.11087 mL	0.07001 mL	5.444	-0.01372	0.82414	0.00075	12.5 s
44:37.2	Data point 44	1.50000 mL	0.10442 mL	0.11101 mL	0.07001 mL	5.696	-0.01715	0.77305	0.00096	13.5 s
45:21.1	Data point 45	1.50000 mL	0.10442 mL	0.11112 mL	0.07001 mL	6.130	-0.01954	0.96881	0.00098	26.5 s
46:18.2	Data point 46	1.50000 mL	0.10442 mL	0.11122 mL	0.07001 mL	6.592	-0.01874	0.90315	0.00097	53.5 s
47:47.4	Data point 47	1.50000 mL	0.10442 mL	0.11129 mL	0.07001 mL	7.084	-0.04097	0.96909	0.00205	Timed out at 59.5 s
49:17.9	Data point 48	1.50000 mL	0.10442 mL	0.11134 mL	0.07001 mL	7.495	-0.05100	0.98620	0.00253	Timed out at 59.5 s
50:48.4	Data point 49	1.50000 mL	0.10442 mL	0.11138 mL	0.07001 mL	7.776	-0.04776	0.98456	0.00238	Timed out at 59.5 s
52:24.0	Data point 50	1.50000 mL	0.10442 mL	0.11145 mL	0.07001 mL	8.250	-0.03292	0.98852	0.00163	Timed out at 59.5 s
54:10.0	Data point 51	1.50000 mL	0.10442 mL	0.11157 mL	0.07001 mL	8.590	-0.00702	0.18474	0.00081	30.0 s
55:15.7	Data point 52	1.50000 mL	0.10442 mL	0.11164 mL	0.07001 mL	8.848	-0.01818	0.90325	0.00095	35.0 s
56:26.4	Data point 53	1.50000 mL	0.10442 mL	0.11174 mL	0.07001 mL	9.055	-0.01929	0.94782	0.00098	19.5 s
57:46.5	Data point 54	1.50000 mL	0.16536 mL	0.11174 mL	0.17001 mL	1.977	-0.01088	0.90338	0.00057	10.0 s
58:32.8	Data point 55	1.50000 mL	0.16536 mL	0.13133 mL	0.17001 mL	2.175	0.01443	0.67056	0.00087	10.0 s
59:08.5	Data point 56	1.50000 mL	0.16536 mL	0.14320 mL	0.17001 mL	2.362	-0.00235	0.19580	0.00026	10.5 s
59:44.6	Data point 57	1.50000 mL	0.16536 mL	0.15104 mL	0.17001 mL	2.563	0.00080	0.04198	0.00019	10.0 s
1:00:20.1	Data point 58	1.50000 mL	0.16536 mL	0.15618 mL	0.17001 mL	2.744	-0.00463	0.54415	0.00031	10.0 s
1:00:55.6	Data point 59	1.50000 mL	0.16536 mL	0.15985 mL	0.17001 mL	2.949	0.00206	0.02453	0.00065	10.0 s
1:01:31.1	Data point 60	1.50000 mL	0.16536 mL	0.16251 mL	0.17001 mL	3.143	-0.00224	0.06525	0.00043	10.0 s
1:02:06.6	Data point 61	1.50000 mL	0.16536 mL	0.16458 mL	0.17001 mL	3.342	-0.00396	0.72084	0.00023	10.0 s
1:02:42.1	Data point 62	1.50000 mL	0.16536 mL	0.16625 mL	0.17001 mL	3.564	0.00587	0.14501	0.00076	10.0 s
1:03:17.5	Data point 63	1.50000 mL	0.16536 mL	0.16752 mL	0.17001 mL	3.761	0.00890	0.28722	0.00082	10.5 s
1:03:53.5	Data point 64	1.50000 mL	0.16536 mL	0.16851 mL	0.17001 mL	3.925	-0.00097	0.01530	0.00039	10.0 s
1:04:49.6	Data point 65	1.50000 mL	0.16536 mL	0.16966 mL	0.17001 mL	4.128	-0.00722	0.41676	0.00055	10.0 s
1:05:40.5	Data point 66	1.50000 mL	0.16536 mL	0.17056 mL	0.17001 mL	4.359	-0.00877	0.21278	0.00094	10.0 s
1:06:31.4	Data point 67	1.50000 mL	0.16536 mL	0.17121 mL	0.17001 mL	4.575	0.01310	0.51315	0.00090	16.0 s
1:07:28.2	Data point 68	1.50000 mL	0.16536 mL	0.17159 mL	0.17001 mL	4.771	-0.01121	0.73701	0.00065	10.5 s
1:08:09.3	Data point 69	1.50000 mL	0.16536 mL	0.17180 mL	0.17001 mL	4.986	-0.00731	0.13298	0.00099	11.0 s
1:08:50.9	Data point 70	1.50000 mL	0.16536 mL	0.17199 mL	0.17001 mL	5.245	-0.00725	0.21815	0.00077	12.0 s
1:09:38.5	Data point 71	1.50000 mL	0.16536 mL	0.17215 mL	0.17001 mL	5.515	-0.01092	0.47619	0.00078	13.0 s
1:10:22.0	Data point 72	1.50000 mL	0.16536 mL	0.17225 mL	0.17001 mL	5.905	-0.01340	0.44094	0.00100	16.5 s
1:11:09.0	Data point 73	1.50000 mL	0.16536 mL	0.17234 mL	0.17001 mL	6.483	-0.01687	0.87993	0.00089	57.5 s
1:12:37.2	Data point 74	1.50000 mL	0.16536 mL	0.17241 mL	0.17001 mL	6.882	-0.04276	0.96454	0.00215	Timed out at 59.5 s
1:14:12.9	Data point 75	1.50000 mL	0.16536 mL	0.17248 mL	0.17001 mL	7.441	-0.07234	0.98643	0.00360	Timed out at 59.5 s
1:15:43.3	Data point 76	1.50000 mL	0.16536 mL	0.17253 mL	0.17001 mL	7.793	-0.06080	0.98083	0.00303	Timed out at 59.5 s
1:17:13.8	Data point 77	1.50000 mL	0.16536 mL	0.17258 mL	0.17001 mL	8.077	-0.04863	0.96800	0.00244	Timed out at 59.5 s
1:18:49.5	Data point 78	1.50000 mL	0.16536 mL	0.17274 mL	0.17001 mL	8.712	-0.01736	0.96206	0.00087	32.5 s
1:20:02.8	Data point 79	1.50000 mL	0.16536 mL	0.17286 mL	0.17001 mL	8.963	-0.01640	0.89684	0.00086	30.0 s
1:21:03.3	Data point 80	1.50000 mL	0.16536 mL	0.17291 mL	0.17001 mL	9.029	-0.00786	0.17453	0.00093	13.5 s
1:21:25.8	Assay volumes	1.50000 mL	0.16536 mL	0.17291 mL	0.17001 mL					

Sample name: **M09_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03001**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 12:18:26 AM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Pion			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	9.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
Titration Pre-Dose				
Titration pre-dose	None			
Assay Medium				
ISA water volume	1.50 mL			
Water added	Automatic			
Partition solvent type	Octanol			
Partition volume	0.030 mL			
Partition solvent added	Automatic			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	120 seconds			
After sonication stir for	5 seconds			
Sample Dissolution				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	50%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	50%			
Titration 2				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.040 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			

Sample name: **M09_octanol** Experiment start time: **3/3/2018 12:18:26 AM**
 Assay name: **pH-metric high logP** Analyst: **Pion**
 Assay ID: **18C-03001** Instrument ID: **T312060**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titration 3				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.100 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
Data Point Stability				
Stir during data point collection	No			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00100 dpH/dt			
Stability timeout after	60 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.111	3/3/2018 12:18:25 AM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus S	0.9988	3/3/2018 12:18:25 AM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus jH	1.0	3/3/2018 12:18:25 AM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus jOH	-0.8	3/3/2018 12:18:25 AM	C:\Sirius_T3\HCl18C02.t3r
Base concentration factor	1.000	3/3/2018 12:18:26 AM	C:\Sirius_T3\KOH18B27.t3r
Acid concentration factor	0.999	3/3/2018 12:18:25 AM	C:\Sirius_T3\HCl18C02.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T312060		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1200361	3/31/2009 5:24:52 AM
Dispenser 0	Water		3/31/2009 5:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	02-06-2018	2/27/2018 10:05:59 AM
Dispenser 2	Acid		3/31/2009 5:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	02-27-2018	2/27/2018 10:27:22 AM
Dispenser 1	Base		3/31/2009 5:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	9/22/2017	2/27/2018 10:21:22 AM
Dispenser 5	Cosolvent		3/31/2009 5:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 5:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	09-26-17	2/7/2018 9:42:01 AM
Port B	Cyclohexane	11-01-17	2/27/2018 10:37:57 AM
Dispenser 3	Buffer		8/3/2010 5:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	2018/01/31	2/28/2018 10:18:04 AM
Dispenser 6	Octanol		10/22/2010 10:52:43 AM

Sample name: **M09_octanol** Experiment start time: **3/3/2018 12:18:26 AM**
 Assay name: **pH-metric high logP** Analyst: **Pion**
 Assay ID: **18C-03001** Instrument ID: **T312060**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	01-31-2018	2/27/2018 9:59:35 AM
Titrator		T3TM1200161	3/31/2009 5:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0923	1/23/2018 2:01:00 PM
E0 calibration	+4.45 mV		3/3/2018 12:18:54 AM
Filling solution	3M KCl	KCL097	3/2/2018 9:43:24 AM
Liquids			
Wash 1	50% IPA:50% Water		3/2/2018 9:45:12 AM
Wash 2	0.5% Triton X-100 in H2O		3/2/2018 9:45:15 AM
Buffer position 1	pH7 Wash		3/2/2018 9:45:18 AM
Buffer position 2	pH 7		3/2/2018 9:45:21 AM
Storage position			3/2/2018 9:44:44 AM
Wash water	7.2e+003 mL	02-27-2018	2/27/2018 9:54:39 AM
Waste	8.3e+003 mL		11/28/2017 10:36:29 AM
Temperature controller			8/5/2010 6:35:13 AM
Turbidity detector			3/31/2009 5:24:45 AM
Spectrometer		074811	11/23/2010 11:22:28 AM
Dip probe		10196	
Wavelength coefficient A0	183.333		
Wavelength coefficient A1	2.21568		
Wavelength coefficient A2	-0.000289308		
Total lamp lit time	120:41:49		11/23/2010 11:22:28 AM
Calibrated on	2/27/2018 10:40:38 AM		
Integration time	40		
Scans averaged	10		
Autoloader		T3AL1200345	11/10/2015 9:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		

Sample name:	M09_octanol	Experiment start time:	3/3/2018 12:18:26 AM
Assay name:	pH-metric high logP	Analyst:	Pion
Assay ID:	18C-03001	Instrument ID:	T312060
Filename:	C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r		

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00

Experiment Log

[2:37] Air gap created for Water (0.15 M KCl)
 [2:37] Air gap created for Acid (0.5 M HCl)
 [2:38] Air gap created for Base (0.5 M KOH)
 [2:38] Air gap released for Water (0.15 M KCl)
 [2:42] Titrator arm moved over Titration position
 [2:42] Titration 1 of 3
 [2:42] Adding initial titrants
 [2:42] Automatically add 1.50000 mL of water
 [3:07] Dispensed 1.500000 mL of Water (0.15 M KCl)
 [3:11] Titrator arm moved over Drain
 [5:52] Titrator arm moved to Titration position
 [5:52] Argon flow rate set to 100
 [5:52] Stirrer speed set to 10
 [5:57] Automatically add 0.03000 mL of Octanol
 [5:58] Dispensed 0.030009 mL of Octanol
 [5:59] Initial pH = 4.70
 [5:59] Iterative adjust 4.70 -> 2.00
 [5:59] pH 4.70 -> 2.00
 [6:01] Air gap released for Acid (0.5 M HCl)
 [6:02] Dispensed 0.046096 mL of Acid (0.5 M HCl)
 [6:07] pH 2.02 -> 2.00
 [6:07] Dispensed 0.001717 mL of Acid (0.5 M HCl)
 [6:12] Holding pH 2.00
 [8:12] Stirrer speed set to 0
 [8:12] Stirrer speed set to 50
 [8:12] Iterative adjust 1.97 -> 2.00
 [8:12] pH 1.97 -> 2.00
 [8:13] Air gap released for Base (0.5 M KOH)
 [8:14] Dispensed 0.003222 mL of Base (0.5 M KOH)
 [9:04] Stirrer speed set to 0
 [9:14] Datapoint id 1 collected
 [9:14] Stirrer speed set to 50
 [9:19] pH 2.00 -> 2.20
 [9:19] Using cautious pH adjust
 [9:19] Dispensed 0.007690 mL of Base (0.5 M KOH)
 [9:24] Stepping pH = 2.08
 [9:25] Dispensed 0.006867 mL of Base (0.5 M KOH)
 [9:30] Stepping pH = 2.18
 [9:30] Dispensed 0.001505 mL of Base (0.5 M KOH)
 [9:35] Stepping pH = 2.20
 [9:50] Stirrer speed set to 0
 [10:00] Datapoint id 2 collected

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03001**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 12:18:26 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[10:00] Charge balance equation is out by -4.5%
[10:00] Stirrer speed set to 50
[10:05] pH 2.21 -> 2.41
[10:05] Using charge balance adjust
[10:06] Dispensed 0.009572 mL of Base (0.5 M KOH)
[10:26] Stirrer speed set to 0
[10:36] Datapoint id 3 collected
[10:36] Charge balance equation is out by -12.3%
[10:36] Stirrer speed set to 50
[10:41] pH 2.39 -> 2.59
[10:41] Using charge balance adjust
[10:41] Dispensed 0.006350 mL of Base (0.5 M KOH)
[11:01] Stirrer speed set to 0
[11:11] Datapoint id 4 collected
[11:11] Charge balance equation is out by -7.1%
[11:11] Stirrer speed set to 50
[11:17] pH 2.58 -> 2.78
[11:17] Using charge balance adjust
[11:17] Dispensed 0.004139 mL of Base (0.5 M KOH)
[11:37] Stirrer speed set to 0
[11:47] Datapoint id 5 collected
[11:47] Charge balance equation is out by -8.6%
[11:47] Stirrer speed set to 50
[11:52] pH 2.77 -> 2.97
[11:52] Using charge balance adjust
[11:52] Dispensed 0.002799 mL of Base (0.5 M KOH)
[12:12] Stirrer speed set to 0
[12:22] Datapoint id 6 collected
[12:22] Charge balance equation is out by -6.9%
[12:22] Stirrer speed set to 50
[12:28] pH 2.97 -> 3.17
[12:28] Using charge balance adjust
[12:28] Dispensed 0.001976 mL of Base (0.5 M KOH)
[12:48] Stirrer speed set to 0
[12:58] Datapoint id 7 collected
[12:58] Charge balance equation is out by 13.6%
[12:58] Stirrer speed set to 50
[13:03] pH 3.20 -> 3.40
[13:03] Using charge balance adjust
[13:03] Dispensed 0.001458 mL of Base (0.5 M KOH)
[13:23] Stirrer speed set to 0
[13:33] Datapoint id 8 collected
[13:33] Charge balance equation is out by 15.2%
[13:33] Stirrer speed set to 50
[13:38] pH 3.44 -> 3.64
[13:38] Using cautious pH adjust
[13:39] Dispensed 0.000611 mL of Base (0.5 M KOH)
[13:44] Stepping pH = 3.54
[13:44] Dispensed 0.000423 mL of Base (0.5 M KOH)
[13:49] Stepping pH = 3.61
[13:49] Dispensed 0.000118 mL of Base (0.5 M KOH)
[13:54] Stepping pH = 3.63
[13:54] Dispensed 0.000071 mL of Base (0.5 M KOH)
[13:59] Stepping pH = 3.64
[14:14] Stirrer speed set to 0
[14:24] Datapoint id 9 collected
[14:24] Charge balance equation is out by 1.1%
[14:24] Stirrer speed set to 50
[14:29] pH 3.63 -> 3.83

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03001**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 12:18:26 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[14:29] Using charge balance adjust
[14:29] Dispensed 0.001176 mL of Base (0.5 M KOH)
[14:50] Stirrer speed set to 0
[15:00] Datapoint id 10 collected
[15:00] Charge balance equation is out by -3.3%
[15:00] Stirrer speed set to 50
[15:05] pH 3.83 -> 4.03
[15:05] Using charge balance adjust
[15:05] Dispensed 0.001105 mL of Base (0.5 M KOH)
[15:25] Stirrer speed set to 0
[15:35] Datapoint id 11 collected
[15:35] Charge balance equation is out by -10.7%
[15:35] Stirrer speed set to 50
[15:40] pH 4.02 -> 4.22
[15:40] Using charge balance adjust
[15:40] Dispensed 0.000988 mL of Base (0.5 M KOH)
[16:01] Stirrer speed set to 0
[16:11] Datapoint id 12 collected
[16:11] Charge balance equation is out by -25.2%
[16:11] Stirrer speed set to 50
[16:16] pH 4.18 -> 4.38
[16:16] Using cautious pH adjust
[16:16] Dispensed 0.000447 mL of Base (0.5 M KOH)
[16:21] Stepping pH = 4.25
[16:21] Dispensed 0.000470 mL of Base (0.5 M KOH)
[16:27] Stepping pH = 4.35
[16:27] Dispensed 0.000118 mL of Base (0.5 M KOH)
[16:32] Stepping pH = 4.34
[16:32] Dispensed 0.000729 mL of Base (0.5 M KOH)
[16:37] Stepping pH = 4.51
[16:52] Stirrer speed set to 0
[17:03] Datapoint id 13 collected
[17:03] Charge balance equation is out by -100.8%
[17:03] Stirrer speed set to 50
[17:08] pH 4.50 -> 4.70
[17:08] Using cautious pH adjust
[17:08] Dispensed 0.000306 mL of Base (0.5 M KOH)
[17:13] Stepping pH = 4.56
[17:13] Dispensed 0.000376 mL of Base (0.5 M KOH)
[17:18] Stepping pH = 4.65
[17:19] Dispensed 0.000141 mL of Base (0.5 M KOH)
[17:24] Stepping pH = 4.67
[17:24] Dispensed 0.000118 mL of Base (0.5 M KOH)
[17:29] Stepping pH = 4.70
[17:44] Stirrer speed set to 0
[17:55] Datapoint id 14 collected
[17:55] Charge balance equation is out by -55.5%
[17:55] Stirrer speed set to 50
[18:00] pH 4.68 -> 4.88
[18:00] Using cautious pH adjust
[18:00] Dispensed 0.000212 mL of Base (0.5 M KOH)
[18:05] Stepping pH = 4.74
[18:05] Dispensed 0.000306 mL of Base (0.5 M KOH)
[18:10] Stepping pH = 4.86
[18:11] Dispensed 0.000047 mL of Base (0.5 M KOH)
[18:16] Stepping pH = 4.86
[18:16] Dispensed 0.000282 mL of Base (0.5 M KOH)
[18:21] Stepping pH = 4.99
[18:36] Stirrer speed set to 0

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
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Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 12:18:26 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[18:48] Datapoint id 15 collected
[18:48] Charge balance equation is out by -89.5%
[18:48] Stirrer speed set to 50
[18:53] pH 4.99 -> 5.19
[18:53] Using cautious pH adjust
[18:53] Dispensed 0.000141 mL of Base (0.5 M KOH)
[18:58] Stepping pH = 5.02
[18:58] Dispensed 0.000235 mL of Base (0.5 M KOH)
[19:03] Stepping pH = 5.15
[19:03] Dispensed 0.000047 mL of Base (0.5 M KOH)
[19:08] Stepping pH = 5.16
[19:09] Dispensed 0.000141 mL of Base (0.5 M KOH)
[19:14] Stepping pH = 5.27
[19:29] Stirrer speed set to 0
[19:42] Datapoint id 16 collected
[19:42] Charge balance equation is out by -110.5%
[19:42] Stirrer speed set to 50
[19:47] pH 5.26 -> 5.46
[19:47] Using cautious pH adjust
[19:47] Dispensed 0.000071 mL of Base (0.5 M KOH)
[19:53] Stepping pH = 5.28
[19:53] Dispensed 0.000212 mL of Base (0.5 M KOH)
[19:58] Stepping pH = 5.48
[20:13] Stirrer speed set to 0
[20:27] Datapoint id 17 collected
[20:27] Charge balance equation is out by -85.7%
[20:27] Stirrer speed set to 50
[20:32] pH 5.48 -> 5.68
[20:32] Using cautious pH adjust
[20:33] Dispensed 0.000047 mL of Base (0.5 M KOH)
[20:38] Stepping pH = 5.48
[20:38] Dispensed 0.000282 mL of Base (0.5 M KOH)
[20:43] Stepping pH = 6.08
[20:58] Stirrer speed set to 0
[21:22] Datapoint id 18 collected
[21:22] Charge balance equation is out by -201.5%
[21:22] Stirrer speed set to 50
[21:27] pH 6.16 -> 6.36
[21:27] Using cautious pH adjust
[21:27] Dispensed 0.000024 mL of Base (0.5 M KOH)
[21:32] Stepping pH = 6.16
[21:32] Dispensed 0.000141 mL of Base (0.5 M KOH)
[21:38] Stepping pH = 6.76
[21:53] Stirrer speed set to 0
[22:48] Datapoint id 19 collected
[22:48] Charge balance equation is out by -210.1%
[22:48] Stirrer speed set to 50
[22:53] pH 6.82 -> 7.02
[22:53] Using cautious pH adjust
[22:53] Dispensed 0.000024 mL of Base (0.5 M KOH)
[22:58] Stepping pH = 6.82
[22:58] Dispensed 0.000071 mL of Base (0.5 M KOH)
[23:03] Stepping pH = 7.05
[23:18] Stirrer speed set to 0
[24:18] Datapoint id 20 collected
[24:18] Charge balance equation is out by -228.7%
[24:18] Stirrer speed set to 50
[24:23] pH 7.20 -> 7.40
[24:23] Using cautious pH adjust

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03001**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 12:18:26 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[24:24] Dispensed 0.000024 mL of Base (0.5 M KOH)
[24:29] Stepping pH = 7.22
[24:29] Dispensed 0.000024 mL of Base (0.5 M KOH)
[24:34] Stepping pH = 7.28
[24:34] Dispensed 0.000024 mL of Base (0.5 M KOH)
[24:39] Stepping pH = 7.54
[24:54] Stirrer speed set to 0
[25:54] Datapoint id 21 collected
[25:54] Charge balance equation is out by -355.4%
[25:54] Stirrer speed set to 50
[25:59] pH 7.96 -> 8.16
[25:59] Using cautious pH adjust
[25:59] Dispensed 0.000024 mL of Base (0.5 M KOH)
[26:04] Stepping pH = 7.99
[26:04] Dispensed 0.000024 mL of Base (0.5 M KOH)
[26:09] Stepping pH = 8.15
[26:24] Stirrer speed set to 0
[27:24] Datapoint id 22 collected
[27:24] Charge balance equation is out by -510.2%
[27:24] Stirrer speed set to 50
[27:30] pH 8.24 -> 8.44
[27:30] Using cautious pH adjust
[27:30] Dispensed 0.000024 mL of Base (0.5 M KOH)
[27:35] Stepping pH = 8.26
[27:35] Dispensed 0.000024 mL of Base (0.5 M KOH)
[27:40] Stepping pH = 8.48
[27:55] Stirrer speed set to 0
[28:46] Datapoint id 23 collected
[28:46] Charge balance equation is out by -341.8%
[28:46] Stirrer speed set to 50
[28:51] pH 8.60 -> 8.80
[28:51] Using cautious pH adjust
[28:51] Dispensed 0.000024 mL of Base (0.5 M KOH)
[28:56] Stepping pH = 8.61
[28:56] Dispensed 0.000024 mL of Base (0.5 M KOH)
[29:02] Stepping pH = 8.77
[29:02] Dispensed 0.000024 mL of Base (0.5 M KOH)
[29:07] Stepping pH = 8.94
[29:22] Stirrer speed set to 0
[29:42] Datapoint id 24 collected
[29:42] Charge balance equation is out by -267.1%
[29:42] Stirrer speed set to 50
[29:47] pH 8.96 -> 9.05
[29:47] Using cautious pH adjust
[29:47] Dispensed 0.000024 mL of Base (0.5 M KOH)
[29:53] Stepping pH = 8.97
[29:53] Dispensed 0.000024 mL of Base (0.5 M KOH)
[29:58] Stepping pH = 9.06
[30:13] Stirrer speed set to 0
[30:37] Datapoint id 25 collected
[30:37] Charge balance equation is out by -171.7%
[30:37] Titration 2 of 3
[30:37] Adding initial titrants
[30:37] Automatically add 0.04000 mL of Octanol
[30:38] Dispensed 0.040005 mL of Octanol
[30:38] Stirrer speed set to 10
[30:39] Stirrer speed set to 55
[30:39] Iterative adjust 9.09 -> 2.00
[30:39] pH 9.09 -> 2.00

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03001**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 12:18:26 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[30:40] Dispensed 0.050376 mL of Acid (0.5 M HCl)
[30:46] pH 2.06 -> 2.00
[30:46] Dispensed 0.006232 mL of Acid (0.5 M HCl)
[31:36] Stirrer speed set to 0
[31:46] Datapoint id 26 collected
[31:46] Stirrer speed set to 55
[31:51] pH 1.99 -> 2.19
[31:51] Using cautious pH adjust
[31:51] Dispensed 0.008561 mL of Base (0.5 M KOH)
[31:57] Stepping pH = 2.08
[31:57] Dispensed 0.006515 mL of Base (0.5 M KOH)
[32:02] Stepping pH = 2.15
[32:02] Dispensed 0.002799 mL of Base (0.5 M KOH)
[32:07] Stepping pH = 2.18
[32:22] Stirrer speed set to 0
[32:32] Datapoint id 27 collected
[32:32] Charge balance equation is out by -4.4%
[32:32] Stirrer speed set to 55
[32:37] pH 2.19 -> 2.39
[32:37] Using charge balance adjust
[32:38] Dispensed 0.010795 mL of Base (0.5 M KOH)
[32:58] Stirrer speed set to 0
[33:08] Datapoint id 28 collected
[33:08] Charge balance equation is out by -0.6%
[33:08] Stirrer speed set to 55
[33:14] pH 2.39 -> 2.59
[33:14] Using charge balance adjust
[33:14] Dispensed 0.006820 mL of Base (0.5 M KOH)
[33:34] Stirrer speed set to 0
[33:45] Datapoint id 29 collected
[33:45] Charge balance equation is out by -14.0%
[33:45] Stirrer speed set to 55
[33:50] pH 2.57 -> 2.77
[33:50] Using charge balance adjust
[33:50] Dispensed 0.004657 mL of Base (0.5 M KOH)
[34:10] Stirrer speed set to 0
[34:20] Datapoint id 30 collected
[34:20] Charge balance equation is out by -11.3%
[34:20] Stirrer speed set to 55
[34:25] pH 2.76 -> 2.96
[34:25] Using charge balance adjust
[34:25] Dispensed 0.003246 mL of Base (0.5 M KOH)
[34:46] Stirrer speed set to 0
[34:56] Datapoint id 31 collected
[34:56] Charge balance equation is out by -10.5%
[34:56] Stirrer speed set to 55
[35:01] pH 2.94 -> 3.14
[35:01] Using charge balance adjust
[35:01] Dispensed 0.002375 mL of Base (0.5 M KOH)
[35:21] Stirrer speed set to 0
[35:32] Datapoint id 32 collected
[35:32] Charge balance equation is out by 29.9%
[35:32] Stirrer speed set to 55
[35:37] pH 3.21 -> 3.41
[35:37] Using cautious pH adjust
[35:37] Dispensed 0.000870 mL of Base (0.5 M KOH)
[35:42] Stepping pH = 3.32
[35:42] Dispensed 0.000517 mL of Base (0.5 M KOH)
[35:47] Stepping pH = 3.39

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03001**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 12:18:26 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[35:47] Dispensed 0.000118 mL of Base (0.5 M KOH)
[35:52] Stepping pH = 3.40
[36:07] Stirrer speed set to 0
[36:18] Datapoint id 33 collected
[36:18] Charge balance equation is out by 13.6%
[36:18] Stirrer speed set to 55
[36:23] pH 3.40 -> 3.60
[36:23] Using charge balance adjust
[36:23] Dispensed 0.001482 mL of Base (0.5 M KOH)
[36:43] Stirrer speed set to 0
[36:53] Datapoint id 34 collected
[36:53] Charge balance equation is out by 4.3%
[36:53] Stirrer speed set to 55
[36:58] pH 3.61 -> 3.81
[36:58] Using charge balance adjust
[36:58] Dispensed 0.001270 mL of Base (0.5 M KOH)
[37:18] Stirrer speed set to 0
[37:28] Datapoint id 35 collected
[37:28] Charge balance equation is out by -15.5%
[37:28] Stirrer speed set to 55
[37:34] pH 3.78 -> 3.98
[37:34] Using cautious pH adjust
[37:34] Dispensed 0.000541 mL of Base (0.5 M KOH)
[37:39] Stepping pH = 3.86
[37:39] Dispensed 0.000541 mL of Base (0.5 M KOH)
[37:44] Stepping pH = 3.95
[37:44] Dispensed 0.000188 mL of Base (0.5 M KOH)
[37:49] Stepping pH = 3.97
[37:49] Dispensed 0.000071 mL of Base (0.5 M KOH)
[37:54] Stepping pH = 3.97
[37:54] Dispensed 0.000212 mL of Base (0.5 M KOH)
[38:00] Stepping pH = 4.01
[38:15] Stirrer speed set to 0
[38:25] Datapoint id 36 collected
[38:25] Charge balance equation is out by -41.9%
[38:25] Stirrer speed set to 55
[38:30] pH 4.01 -> 4.21
[38:30] Using cautious pH adjust
[38:30] Dispensed 0.000423 mL of Base (0.5 M KOH)
[38:35] Stepping pH = 4.09
[38:35] Dispensed 0.000400 mL of Base (0.5 M KOH)
[38:41] Stepping pH = 4.17
[38:41] Dispensed 0.000188 mL of Base (0.5 M KOH)
[38:46] Stepping pH = 4.20
[38:46] Dispensed 0.000071 mL of Base (0.5 M KOH)
[38:51] Stepping pH = 4.21
[39:06] Stirrer speed set to 0
[39:16] Datapoint id 37 collected
[39:16] Charge balance equation is out by -27.1%
[39:16] Stirrer speed set to 55
[39:21] pH 4.21 -> 4.41
[39:21] Using cautious pH adjust
[39:21] Dispensed 0.000329 mL of Base (0.5 M KOH)
[39:26] Stepping pH = 4.28
[39:26] Dispensed 0.000306 mL of Base (0.5 M KOH)
[39:31] Stepping pH = 4.36
[39:31] Dispensed 0.000141 mL of Base (0.5 M KOH)
[39:37] Stepping pH = 4.39
[39:37] Dispensed 0.000047 mL of Base (0.5 M KOH)

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03001**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 12:18:26 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[39:42] Stepping pH = 4.40
[39:42] Dispensed 0.000071 mL of Base (0.5 M KOH)
[39:47] Stepping pH = 4.41
[40:02] Stirrer speed set to 0
[40:12] Datapoint id 38 collected
[40:12] Charge balance equation is out by -35.9%
[40:12] Stirrer speed set to 55
[40:17] pH 4.41 -> 4.61
[40:17] Using cautious pH adjust
[40:17] Dispensed 0.000235 mL of Base (0.5 M KOH)
[40:22] Stepping pH = 4.48
[40:22] Dispensed 0.000259 mL of Base (0.5 M KOH)
[40:27] Stepping pH = 4.57
[40:28] Dispensed 0.000094 mL of Base (0.5 M KOH)
[40:33] Stepping pH = 4.59
[40:33] Dispensed 0.000071 mL of Base (0.5 M KOH)
[40:38] Stepping pH = 4.60
[40:53] Stirrer speed set to 0
[41:03] Datapoint id 39 collected
[41:03] Charge balance equation is out by -42.4%
[41:03] Stirrer speed set to 55
[41:08] pH 4.61 -> 4.81
[41:08] Using cautious pH adjust
[41:08] Dispensed 0.000165 mL of Base (0.5 M KOH)
[41:13] Stepping pH = 4.66
[41:13] Dispensed 0.000212 mL of Base (0.5 M KOH)
[41:18] Stepping pH = 4.76
[41:18] Dispensed 0.000071 mL of Base (0.5 M KOH)
[41:24] Stepping pH = 4.78
[41:24] Dispensed 0.000094 mL of Base (0.5 M KOH)
[41:29] Stepping pH = 4.82
[41:44] Stirrer speed set to 0
[41:54] Datapoint id 40 collected
[41:54] Charge balance equation is out by -63.5%
[41:54] Stirrer speed set to 55
[41:59] pH 4.83 -> 5.03
[41:59] Using cautious pH adjust
[41:59] Dispensed 0.000094 mL of Base (0.5 M KOH)
[42:05] Stepping pH = 4.86
[42:05] Dispensed 0.000235 mL of Base (0.5 M KOH)
[42:10] Stepping pH = 5.02
[42:10] Dispensed 0.000024 mL of Base (0.5 M KOH)
[42:15] Stepping pH = 5.03
[42:30] Stirrer speed set to 0
[42:41] Datapoint id 41 collected
[42:41] Charge balance equation is out by -73.8%
[42:41] Stirrer speed set to 55
[42:46] pH 5.04 -> 5.24
[42:46] Using cautious pH adjust
[42:46] Dispensed 0.000071 mL of Base (0.5 M KOH)
[42:51] Stepping pH = 5.06
[42:51] Dispensed 0.000165 mL of Base (0.5 M KOH)
[42:56] Stepping pH = 5.23
[43:12] Stirrer speed set to 0
[43:23] Datapoint id 42 collected
[43:23] Charge balance equation is out by -73.2%
[43:23] Stirrer speed set to 55
[43:28] pH 5.25 -> 5.45
[43:28] Using cautious pH adjust

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03001**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 12:18:26 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[43:28] Dispensed 0.000047 mL of Base (0.5 M KOH)
[43:33] Stepping pH = 5.25
[43:33] Dispensed 0.000141 mL of Base (0.5 M KOH)
[43:39] Stepping pH = 5.44
[43:54] Stirrer speed set to 0
[44:06] Datapoint id 43 collected
[44:06] Charge balance equation is out by -97.6%
[44:06] Stirrer speed set to 55
[44:11] pH 5.47 -> 5.67
[44:11] Using cautious pH adjust
[44:11] Dispensed 0.000047 mL of Base (0.5 M KOH)
[44:16] Stepping pH = 5.48
[44:17] Dispensed 0.000094 mL of Base (0.5 M KOH)
[44:22] Stepping pH = 5.69
[44:37] Stirrer speed set to 0
[44:50] Datapoint id 44 collected
[44:50] Charge balance equation is out by -89.8%
[44:50] Stirrer speed set to 55
[44:55] pH 5.73 -> 5.93
[44:55] Using cautious pH adjust
[44:55] Dispensed 0.000024 mL of Base (0.5 M KOH)
[45:00] Stepping pH = 5.74
[45:00] Dispensed 0.000094 mL of Base (0.5 M KOH)
[45:06] Stepping pH = 6.11
[45:21] Stirrer speed set to 0
[45:47] Datapoint id 45 collected
[45:47] Charge balance equation is out by -93.6%
[45:47] Stirrer speed set to 55
[45:52] pH 6.19 -> 6.39
[45:52] Using cautious pH adjust
[45:52] Dispensed 0.000024 mL of Base (0.5 M KOH)
[45:57] Stepping pH = 6.20
[45:57] Dispensed 0.000071 mL of Base (0.5 M KOH)
[46:03] Stepping pH = 6.56
[46:18] Stirrer speed set to 0
[47:11] Datapoint id 46 collected
[47:11] Charge balance equation is out by -89.9%
[47:11] Stirrer speed set to 55
[47:16] pH 6.72 -> 6.92
[47:16] Using cautious pH adjust
[47:16] Dispensed 0.000024 mL of Base (0.5 M KOH)
[47:22] Stepping pH = 6.76
[47:22] Dispensed 0.000024 mL of Base (0.5 M KOH)
[47:27] Stepping pH = 6.87
[47:27] Dispensed 0.000024 mL of Base (0.5 M KOH)
[47:32] Stepping pH = 7.07
[47:47] Stirrer speed set to 0
[48:47] Datapoint id 47 collected
[48:47] Charge balance equation is out by -117.3%
[48:47] Stirrer speed set to 55
[48:52] pH 7.14 -> 7.34
[48:52] Using cautious pH adjust
[48:52] Dispensed 0.000024 mL of Base (0.5 M KOH)
[48:57] Stepping pH = 7.19
[48:57] Dispensed 0.000024 mL of Base (0.5 M KOH)
[49:02] Stepping pH = 7.37
[49:17] Stirrer speed set to 0
[50:17] Datapoint id 48 collected
[50:17] Charge balance equation is out by -157.7%

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03001**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 12:18:26 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[50:17] Stirrer speed set to 55
[50:23] pH 7.40 -> 7.60
[50:23] Using cautious pH adjust
[50:23] Dispensed 0.000024 mL of Base (0.5 M KOH)
[50:28] Stepping pH = 7.40
[50:28] Dispensed 0.000024 mL of Base (0.5 M KOH)
[50:33] Stepping pH = 7.65
[50:48] Stirrer speed set to 0
[51:48] Datapoint id 49 collected
[51:48] Charge balance equation is out by -351.7%
[51:48] Stirrer speed set to 55
[51:53] pH 7.81 -> 8.01
[51:53] Using cautious pH adjust
[51:53] Dispensed 0.000024 mL of Base (0.5 M KOH)
[51:58] Stepping pH = 7.82
[51:58] Dispensed 0.000024 mL of Base (0.5 M KOH)
[52:03] Stepping pH = 7.91
[52:03] Dispensed 0.000024 mL of Base (0.5 M KOH)
[52:08] Stepping pH = 8.19
[52:24] Stirrer speed set to 0
[53:24] Datapoint id 50 collected
[53:24] Charge balance equation is out by -782.1%
[53:24] Stirrer speed set to 55
[53:29] pH 8.25 -> 8.45
[53:29] Using cautious pH adjust
[53:29] Dispensed 0.000024 mL of Base (0.5 M KOH)
[53:34] Stepping pH = 8.27
[53:34] Dispensed 0.000024 mL of Base (0.5 M KOH)
[53:39] Stepping pH = 8.31
[53:39] Dispensed 0.000024 mL of Base (0.5 M KOH)
[53:44] Stepping pH = 8.38
[53:44] Dispensed 0.000024 mL of Base (0.5 M KOH)
[53:49] Stepping pH = 8.42
[53:49] Dispensed 0.000024 mL of Base (0.5 M KOH)
[53:54] Stepping pH = 8.58
[54:10] Stirrer speed set to 0
[54:40] Datapoint id 51 collected
[54:40] Charge balance equation is out by -941.0%
[54:40] Stirrer speed set to 55
[54:45] pH 8.62 -> 8.82
[54:45] Using cautious pH adjust
[54:45] Dispensed 0.000024 mL of Base (0.5 M KOH)
[54:50] Stepping pH = 8.65
[54:50] Dispensed 0.000024 mL of Base (0.5 M KOH)
[54:55] Stepping pH = 8.73
[54:55] Dispensed 0.000024 mL of Base (0.5 M KOH)
[55:00] Stepping pH = 8.85
[55:15] Stirrer speed set to 0
[55:50] Datapoint id 52 collected
[55:50] Charge balance equation is out by -223.8%
[55:50] Stirrer speed set to 55
[55:55] pH 8.86 -> 9.05
[55:55] Using cautious pH adjust
[55:55] Dispensed 0.000024 mL of Base (0.5 M KOH)
[56:01] Stepping pH = 8.86
[56:01] Dispensed 0.000047 mL of Base (0.5 M KOH)
[56:06] Stepping pH = 8.99
[56:06] Dispensed 0.000024 mL of Base (0.5 M KOH)
[56:11] Stepping pH = 9.06

Sample name: **M09_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03001**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 12:18:26 AM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Experiment Log (continued)

[56:26] Stirrer speed set to 0
 [56:45] Datapoint id 53 collected
 [56:45] Charge balance equation is out by -177.4%
 [56:45] Titration 3 of 3
 [56:45] Adding initial titrants
 [56:45] Automatically add 0.10000 mL of Octanol
 [56:48] Dispensed 0.100000 mL of Octanol
 [56:48] Stirrer speed set to 10
 [56:49] Stirrer speed set to 60
 [56:49] Iterative adjust 9.06 -> 2.00
 [56:49] pH 9.06 -> 2.00
 [56:50] Dispensed 0.053293 mL of Acid (0.5 M HCl)
 [56:55] pH 2.07 -> 2.00
 [56:56] Dispensed 0.007643 mL of Acid (0.5 M HCl)
 [57:46] Stirrer speed set to 0
 [57:56] Datapoint id 54 collected
 [57:56] Stirrer speed set to 60
 [58:01] pH 1.98 -> 2.18
 [58:01] Using cautious pH adjust
 [58:01] Dispensed 0.009431 mL of Base (0.5 M KOH)
 [58:07] Stepping pH = 2.06
 [58:07] Dispensed 0.007902 mL of Base (0.5 M KOH)
 [58:12] Stepping pH = 2.15
 [58:12] Dispensed 0.002258 mL of Base (0.5 M KOH)
 [58:17] Stepping pH = 2.17
 [58:32] Stirrer speed set to 0
 [58:42] Datapoint id 55 collected
 [58:42] Charge balance equation is out by -3.9%
 [58:42] Stirrer speed set to 60
 [58:47] pH 2.18 -> 2.38
 [58:47] Using charge balance adjust
 [58:48] Dispensed 0.011877 mL of Base (0.5 M KOH)
 [59:08] Stirrer speed set to 0
 [59:19] Datapoint id 56 collected
 [59:19] Charge balance equation is out by -8.4%
 [59:19] Stirrer speed set to 60
 [59:24] pH 2.37 -> 2.57
 [59:24] Using charge balance adjust
 [59:24] Dispensed 0.007832 mL of Base (0.5 M KOH)
 [59:44] Stirrer speed set to 0
 [59:54] Datapoint id 57 collected
 [59:54] Charge balance equation is out by -1.8%
 [59:54] Stirrer speed set to 60
 [59:59] pH 2.57 -> 2.77
 [59:59] Using charge balance adjust
 [59:59] Dispensed 0.005151 mL of Base (0.5 M KOH)
 [1:00:20] Stirrer speed set to 0
 [1:00:30] Datapoint id 58 collected
 [1:00:30] Charge balance equation is out by -13.0%
 [1:00:30] Stirrer speed set to 60
 [1:00:35] pH 2.75 -> 2.95
 [1:00:35] Using charge balance adjust
 [1:00:35] Dispensed 0.003669 mL of Base (0.5 M KOH)
 [1:00:55] Stirrer speed set to 0
 [1:01:05] Datapoint id 59 collected
 [1:01:05] Charge balance equation is out by -1.4%
 [1:01:05] Stirrer speed set to 60
 [1:01:10] pH 2.96 -> 3.16
 [1:01:10] Using charge balance adjust

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03001**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 12:18:26 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:01:10] Dispensed 0.002658 mL of Base (0.5 M KOH)
[1:01:31] Stirrer speed set to 0
[1:01:41] Datapoint id 60 collected
[1:01:41] Charge balance equation is out by -7.0%
[1:01:41] Stirrer speed set to 60
[1:01:46] pH 3.15 -> 3.35
[1:01:46] Using charge balance adjust
[1:01:46] Dispensed 0.002070 mL of Base (0.5 M KOH)
[1:02:06] Stirrer speed set to 0
[1:02:16] Datapoint id 61 collected
[1:02:16] Charge balance equation is out by -2.9%
[1:02:16] Stirrer speed set to 60
[1:02:21] pH 3.35 -> 3.55
[1:02:21] Using charge balance adjust
[1:02:21] Dispensed 0.001670 mL of Base (0.5 M KOH)
[1:02:42] Stirrer speed set to 0
[1:02:52] Datapoint id 62 collected
[1:02:52] Charge balance equation is out by 8.9%
[1:02:52] Stirrer speed set to 60
[1:02:57] pH 3.57 -> 3.77
[1:02:57] Using charge balance adjust
[1:02:57] Dispensed 0.001270 mL of Base (0.5 M KOH)
[1:03:17] Stirrer speed set to 0
[1:03:28] Datapoint id 63 collected
[1:03:28] Charge balance equation is out by -5.5%
[1:03:28] Stirrer speed set to 60
[1:03:33] pH 3.77 -> 3.97
[1:03:33] Using charge balance adjust
[1:03:33] Dispensed 0.000988 mL of Base (0.5 M KOH)
[1:03:53] Stirrer speed set to 0
[1:04:03] Datapoint id 64 collected
[1:04:03] Charge balance equation is out by -21.8%
[1:04:03] Stirrer speed set to 60
[1:04:08] pH 3.93 -> 4.13
[1:04:08] Using cautious pH adjust
[1:04:08] Dispensed 0.000376 mL of Base (0.5 M KOH)
[1:04:13] Stepping pH = 4.00
[1:04:13] Dispensed 0.000423 mL of Base (0.5 M KOH)
[1:04:19] Stepping pH = 4.08
[1:04:19] Dispensed 0.000188 mL of Base (0.5 M KOH)
[1:04:24] Stepping pH = 4.11
[1:04:24] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:04:29] Stepping pH = 4.12
[1:04:29] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:04:34] Stepping pH = 4.13
[1:04:49] Stirrer speed set to 0
[1:04:59] Datapoint id 65 collected
[1:04:59] Charge balance equation is out by -52.8%
[1:04:59] Stirrer speed set to 60
[1:05:04] pH 4.14 -> 4.34
[1:05:04] Using cautious pH adjust
[1:05:04] Dispensed 0.000259 mL of Base (0.5 M KOH)
[1:05:09] Stepping pH = 4.20
[1:05:09] Dispensed 0.000329 mL of Base (0.5 M KOH)
[1:05:15] Stepping pH = 4.28
[1:05:15] Dispensed 0.000141 mL of Base (0.5 M KOH)
[1:05:20] Stepping pH = 4.30
[1:05:20] Dispensed 0.000165 mL of Base (0.5 M KOH)
[1:05:25] Stepping pH = 4.36

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03001**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 12:18:26 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:05:40] Stirrer speed set to 0
[1:05:50] Datapoint id 66 collected
[1:05:50] Charge balance equation is out by -68.3%
[1:05:50] Stirrer speed set to 60
[1:05:55] pH 4.36 -> 4.56
[1:05:55] Using cautious pH adjust
[1:05:55] Dispensed 0.000165 mL of Base (0.5 M KOH)
[1:06:00] Stepping pH = 4.40
[1:06:00] Dispensed 0.000353 mL of Base (0.5 M KOH)
[1:06:06] Stepping pH = 4.54
[1:06:06] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:06:11] Stepping pH = 4.54
[1:06:11] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:06:16] Stepping pH = 4.57
[1:06:31] Stirrer speed set to 0
[1:06:47] Datapoint id 67 collected
[1:06:47] Charge balance equation is out by -89.4%
[1:06:47] Stirrer speed set to 60
[1:06:52] pH 4.59 -> 4.79
[1:06:52] Using cautious pH adjust
[1:06:52] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:06:57] Stepping pH = 4.63
[1:06:57] Dispensed 0.000188 mL of Base (0.5 M KOH)
[1:07:02] Stepping pH = 4.76
[1:07:02] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:07:07] Stepping pH = 4.76
[1:07:08] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:07:13] Stepping pH = 4.78
[1:07:28] Stirrer speed set to 0
[1:07:38] Datapoint id 68 collected
[1:07:38] Charge balance equation is out by -71.7%
[1:07:38] Stirrer speed set to 60
[1:07:43] pH 4.79 -> 4.99
[1:07:43] Using cautious pH adjust
[1:07:43] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:07:49] Stepping pH = 4.82
[1:07:49] Dispensed 0.000141 mL of Base (0.5 M KOH)
[1:07:54] Stepping pH = 4.99
[1:08:09] Stirrer speed set to 0
[1:08:20] Datapoint id 69 collected
[1:08:20] Charge balance equation is out by -48.7%
[1:08:20] Stirrer speed set to 60
[1:08:25] pH 5.01 -> 5.21
[1:08:25] Using cautious pH adjust
[1:08:25] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:08:30] Stepping pH = 5.01
[1:08:30] Dispensed 0.000141 mL of Base (0.5 M KOH)
[1:08:35] Stepping pH = 5.24
[1:08:50] Stirrer speed set to 0
[1:09:02] Datapoint id 70 collected
[1:09:02] Charge balance equation is out by -94.7%
[1:09:02] Stirrer speed set to 60
[1:09:07] pH 5.27 -> 5.47
[1:09:07] Using cautious pH adjust
[1:09:07] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:09:13] Stepping pH = 5.27
[1:09:13] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:09:18] Stepping pH = 5.39
[1:09:18] Dispensed 0.000047 mL of Base (0.5 M KOH)

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03001**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 12:18:26 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:09:23] Stepping pH = 5.50
[1:09:38] Stirrer speed set to 0
[1:09:51] Datapoint id 71 collected
[1:09:51] Charge balance equation is out by -168.0%
[1:09:51] Stirrer speed set to 60
[1:09:56] pH 5.56 -> 5.76
[1:09:56] Using cautious pH adjust
[1:09:56] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:10:01] Stepping pH = 5.58
[1:10:01] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:10:06] Stepping pH = 5.86
[1:10:22] Stirrer speed set to 0
[1:10:38] Datapoint id 72 collected
[1:10:38] Charge balance equation is out by -88.7%
[1:10:38] Stirrer speed set to 60
[1:10:43] pH 5.96 -> 6.16
[1:10:43] Using cautious pH adjust
[1:10:43] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:10:48] Stepping pH = 5.98
[1:10:48] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:10:53] Stepping pH = 6.55
[1:11:09] Stirrer speed set to 0
[1:12:06] Datapoint id 73 collected
[1:12:06] Charge balance equation is out by -84.8%
[1:12:06] Stirrer speed set to 60
[1:12:11] pH 6.50 -> 6.70
[1:12:11] Using cautious pH adjust
[1:12:11] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:12:17] Stepping pH = 6.52
[1:12:17] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:12:22] Stepping pH = 6.85
[1:12:37] Stirrer speed set to 0
[1:13:37] Datapoint id 74 collected
[1:13:37] Charge balance equation is out by -88.4%
[1:13:37] Stirrer speed set to 60
[1:13:42] pH 6.98 -> 7.18
[1:13:42] Using cautious pH adjust
[1:13:42] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:13:47] Stepping pH = 7.04
[1:13:47] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:13:52] Stepping pH = 7.14
[1:13:52] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:13:57] Stepping pH = 7.42
[1:14:12] Stirrer speed set to 0
[1:15:12] Datapoint id 75 collected
[1:15:12] Charge balance equation is out by -161.4%
[1:15:12] Stirrer speed set to 60
[1:15:18] pH 7.51 -> 7.71
[1:15:18] Using cautious pH adjust
[1:15:18] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:15:23] Stepping pH = 7.56
[1:15:23] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:15:28] Stepping pH = 7.71
[1:15:43] Stirrer speed set to 0
[1:16:43] Datapoint id 76 collected
[1:16:43] Charge balance equation is out by -306.0%
[1:16:43] Stirrer speed set to 60
[1:16:48] pH 7.94 -> 8.14
[1:16:48] Using cautious pH adjust

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03001**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03001_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 12:18:26 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:16:48] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:16:53] Stepping pH = 8.00
[1:16:53] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:16:58] Stepping pH = 8.19
[1:17:13] Stirrer speed set to 0
[1:18:13] Datapoint id 77 collected
[1:18:13] Charge balance equation is out by -415.5%
[1:18:13] Stirrer speed set to 60
[1:18:18] pH 8.04 -> 8.24
[1:18:18] Using cautious pH adjust
[1:18:19] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:18:24] Stepping pH = 8.02
[1:18:24] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:18:29] Stepping pH = 8.01
[1:18:29] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:18:34] Stepping pH = 8.74
[1:18:49] Stirrer speed set to 0
[1:19:22] Datapoint id 78 collected
[1:19:22] Charge balance equation is out by -1,836.6%
[1:19:22] Stirrer speed set to 60
[1:19:27] pH 8.74 -> 8.94
[1:19:27] Using cautious pH adjust
[1:19:27] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:19:32] Stepping pH = 8.74
[1:19:32] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:19:37] Stepping pH = 8.85
[1:19:37] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:19:42] Stepping pH = 8.90
[1:19:42] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:19:47] Stepping pH = 8.96
[1:20:02] Stirrer speed set to 0
[1:20:32] Datapoint id 79 collected
[1:20:32] Charge balance equation is out by -287.6%
[1:20:32] Stirrer speed set to 60
[1:20:37] pH 8.98 -> 9.05
[1:20:37] Using cautious pH adjust
[1:20:38] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:20:43] Stepping pH = 8.99
[1:20:43] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:20:48] Stepping pH = 9.02
[1:21:03] Stirrer speed set to 0
[1:21:16] Datapoint id 80 collected
[1:21:16] Charge balance equation is out by -194.9%
[1:21:16] Argon flow rate set to 0
[1:21:20] Titrator arm moved over Titration position